Elucidation of A Low Spin Cobalt(II) System in a Distorted Tetrahedral Geometry

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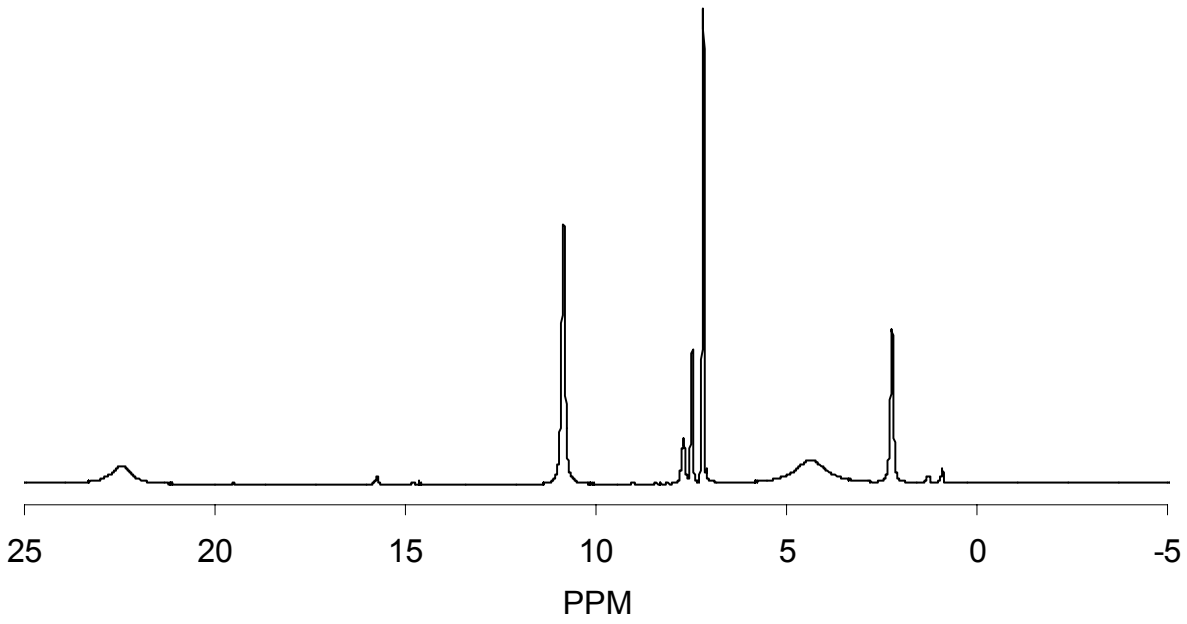
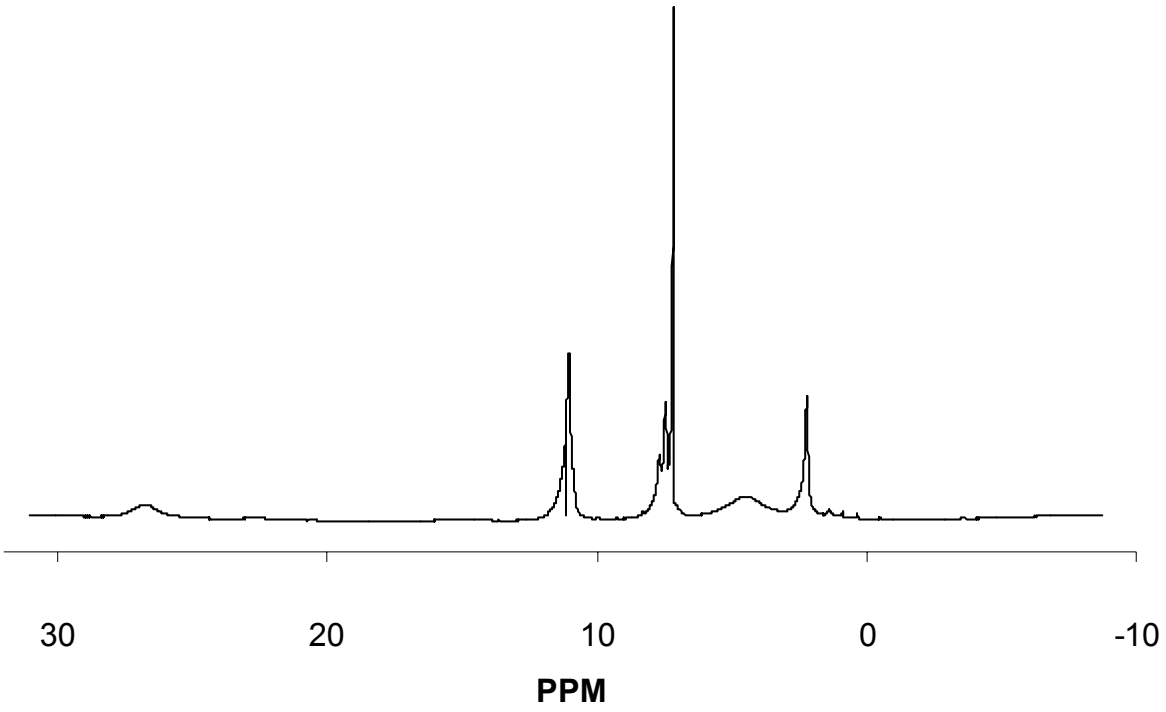
I.

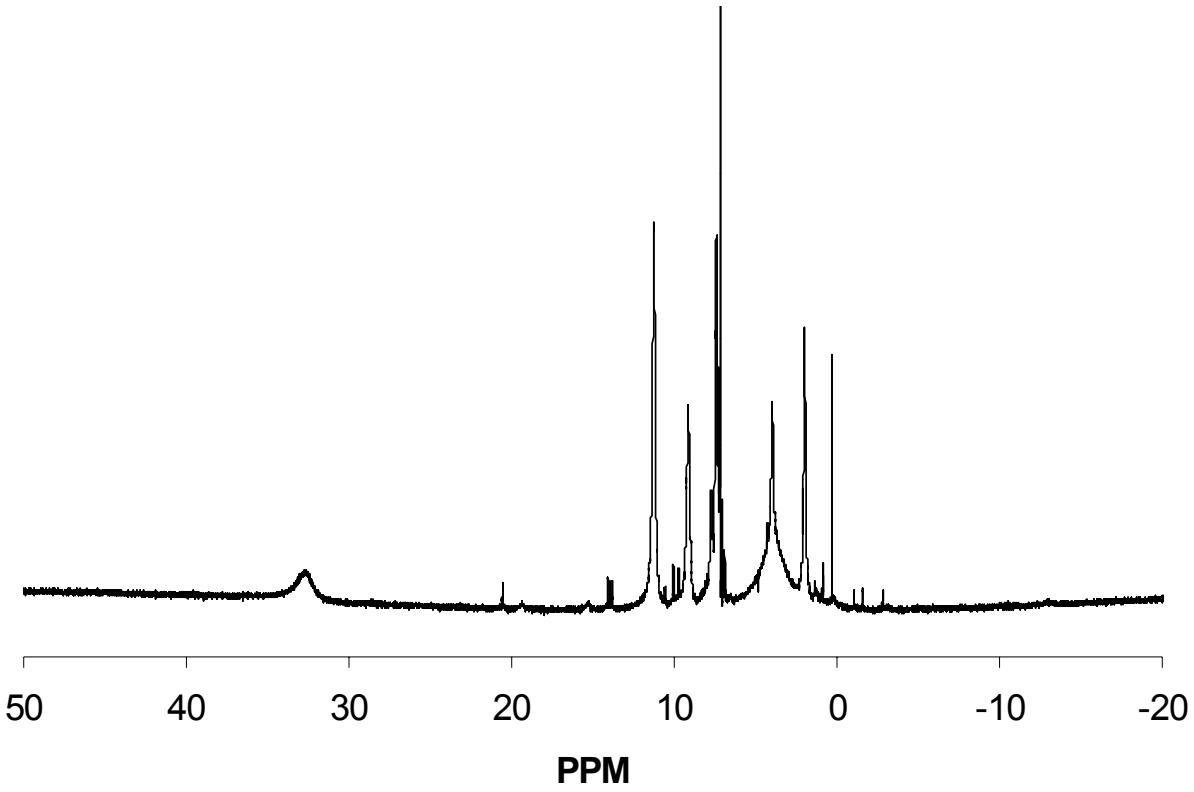
[$PhBP_3$]CoI, (1)



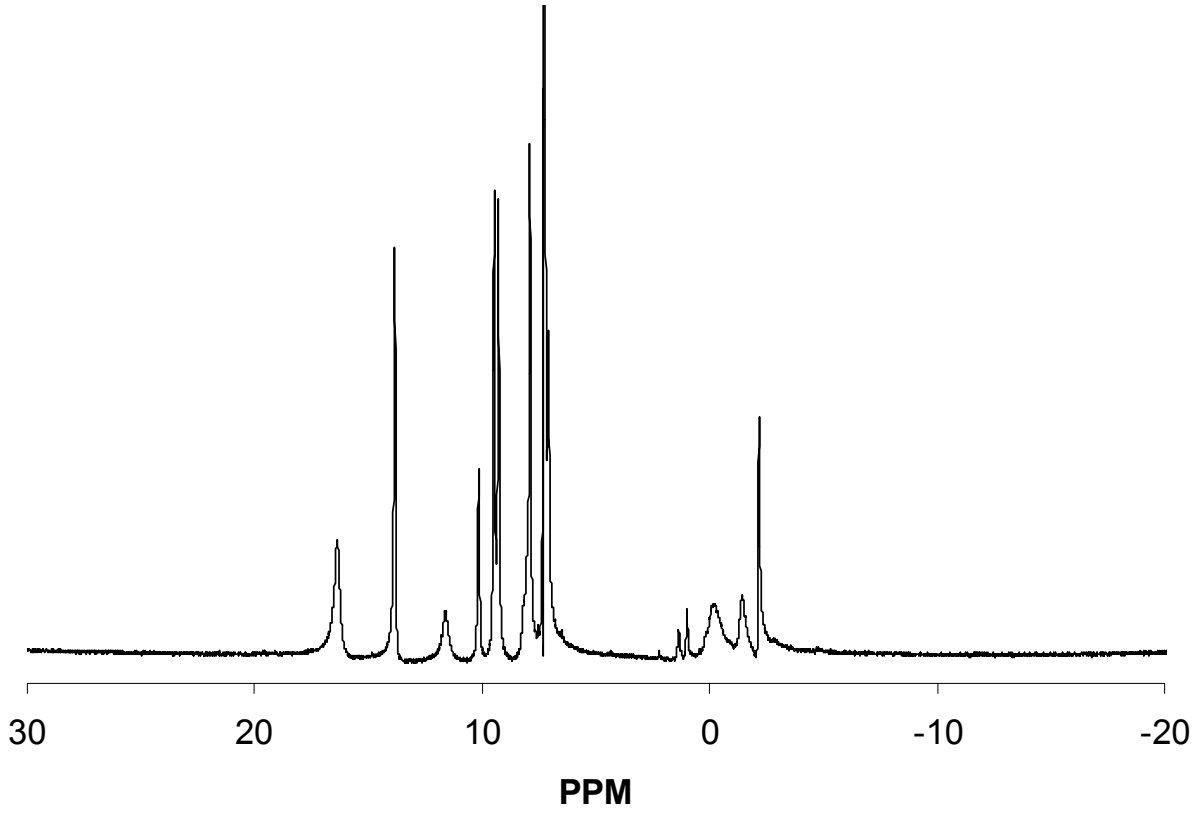
{[PhBP$_3$]Co(μ-Br)}$_2$, (2)



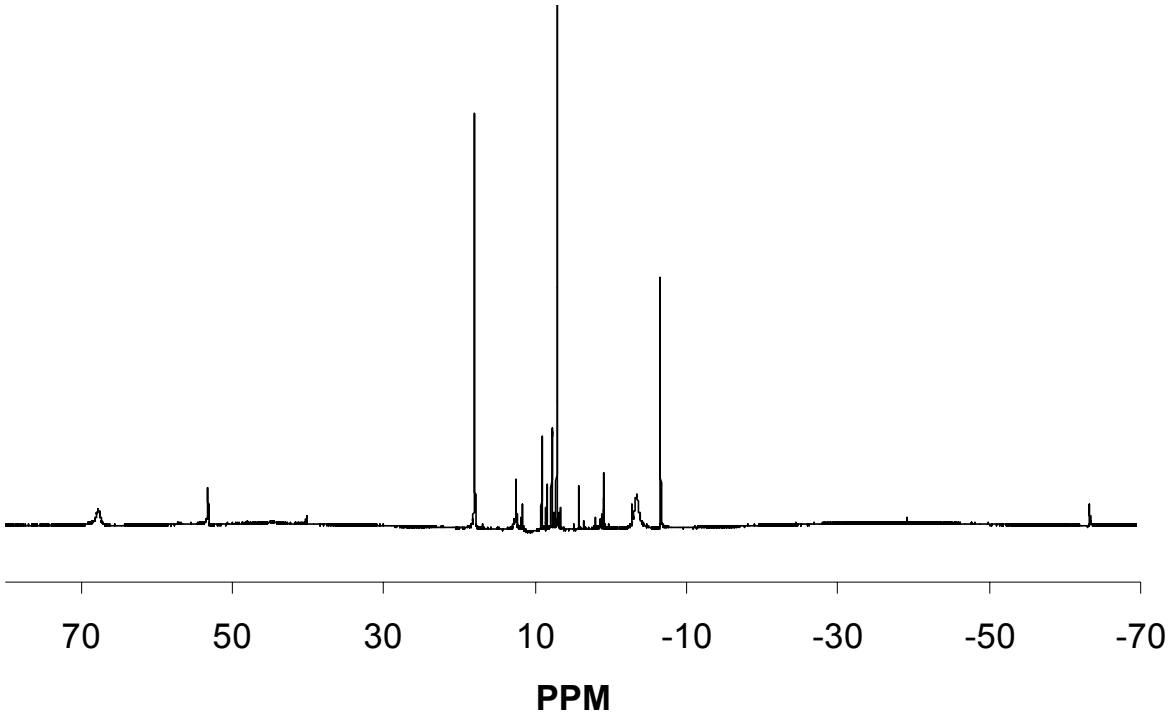
{[PhBP$_3$]Co(μ-Cl)}$_2$, (3)



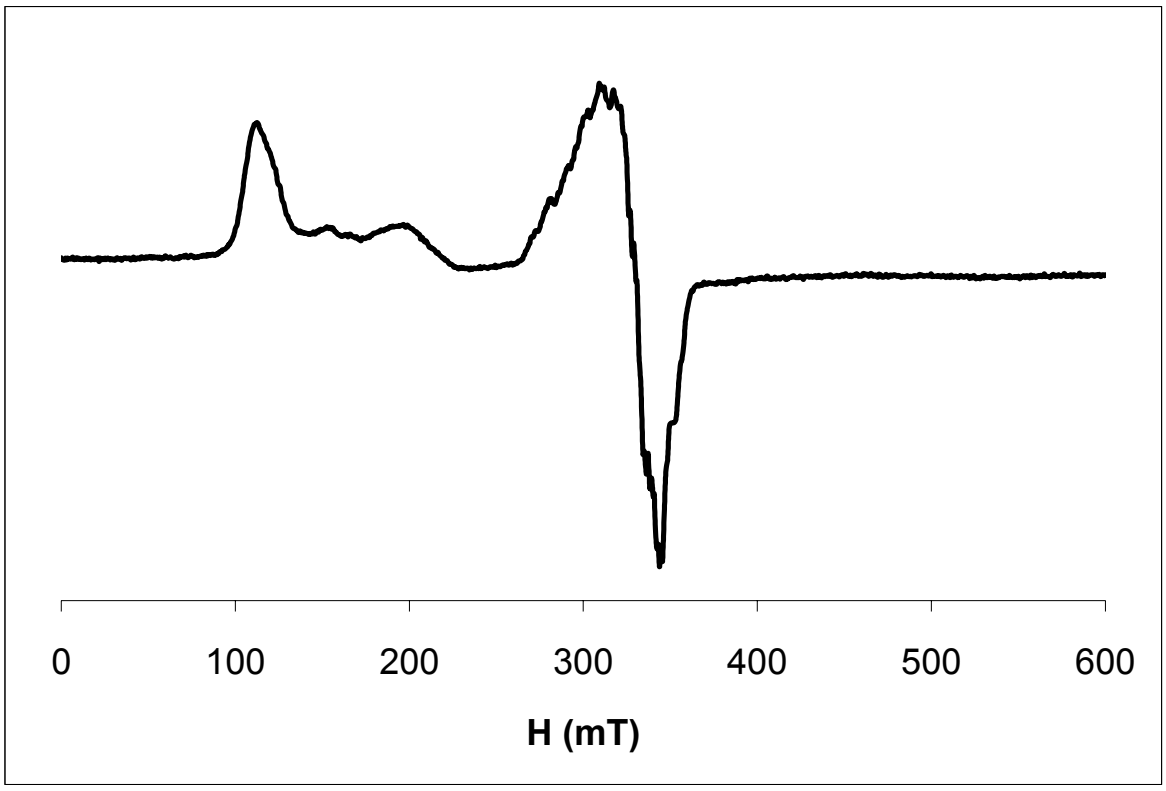
[PhB($CH_2P(O)Ph_2$)$_2$(CH_2PPh_2)]CoI, (4)



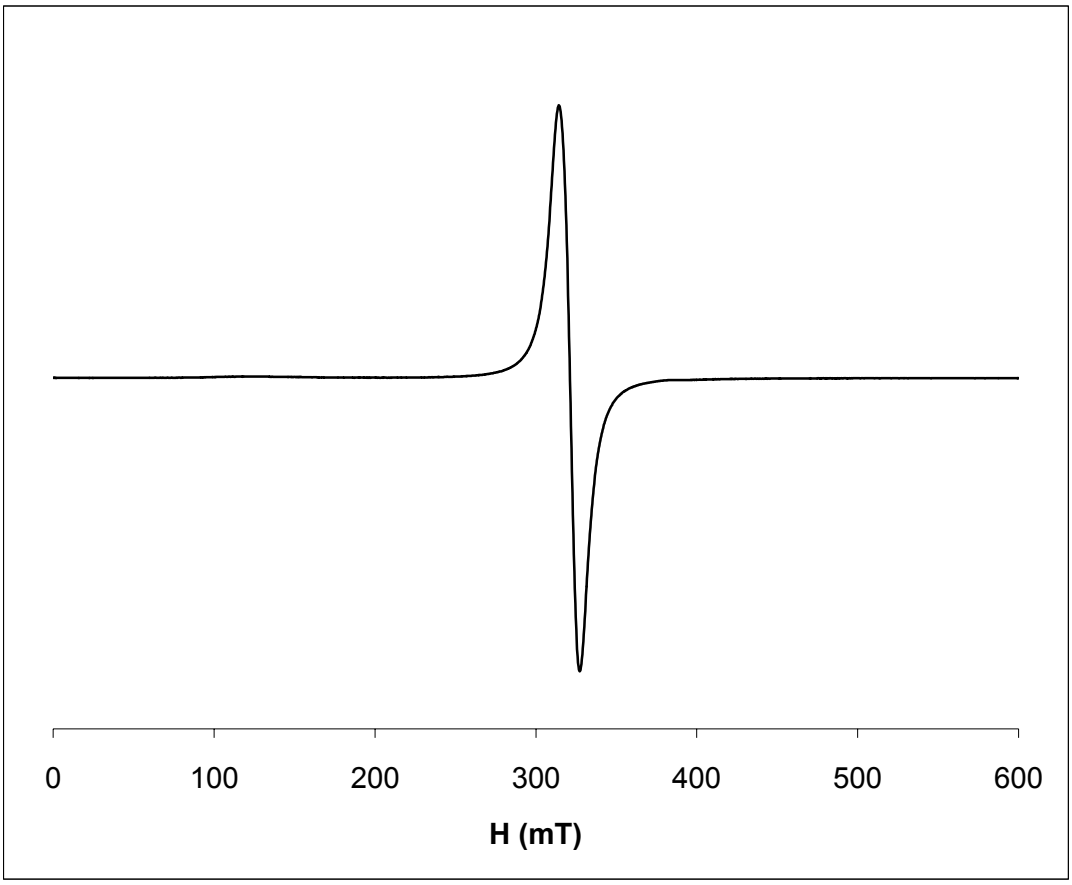
[PhBP$_3$]Co(O-2,6-dimethylphenyl), (5)



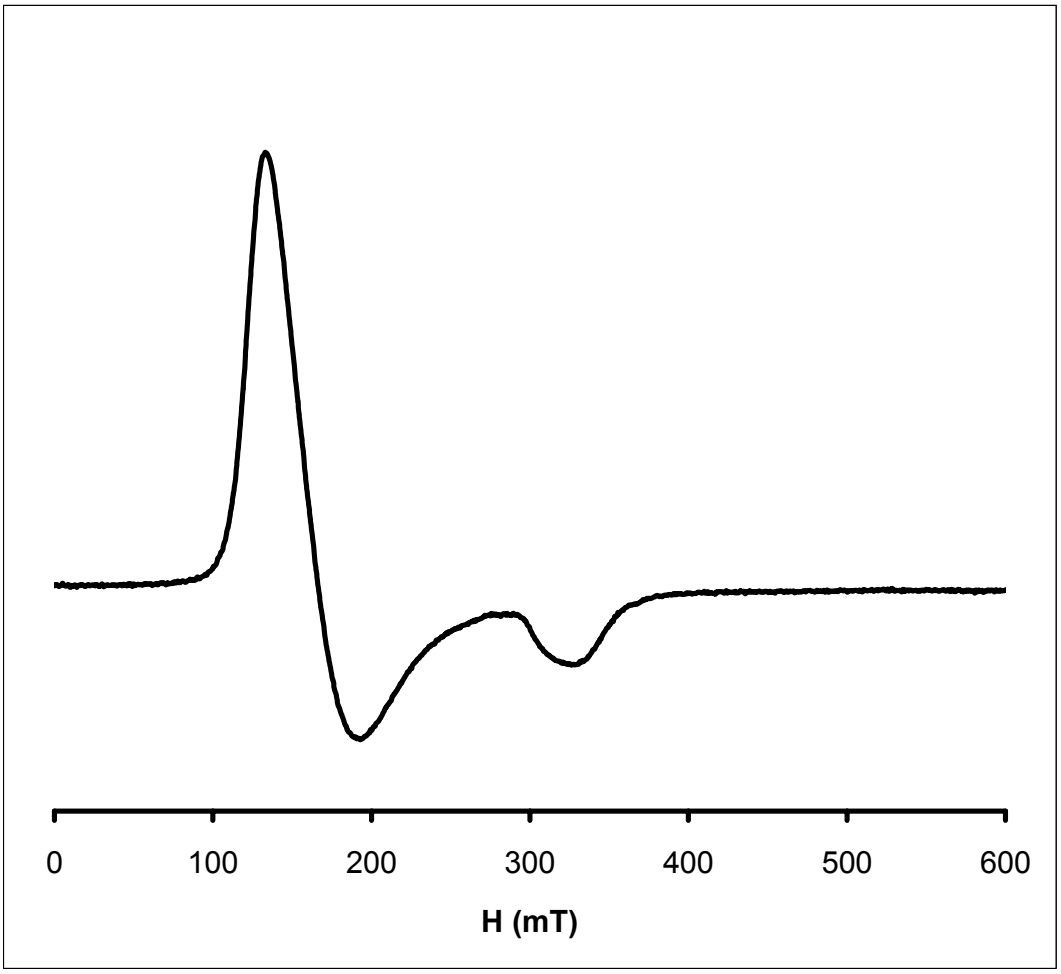
II. EPR spectrum of [$PhBP_3$]Co(O-2,6-dimethylphenyl) (5) (toluene glass, 10 K).



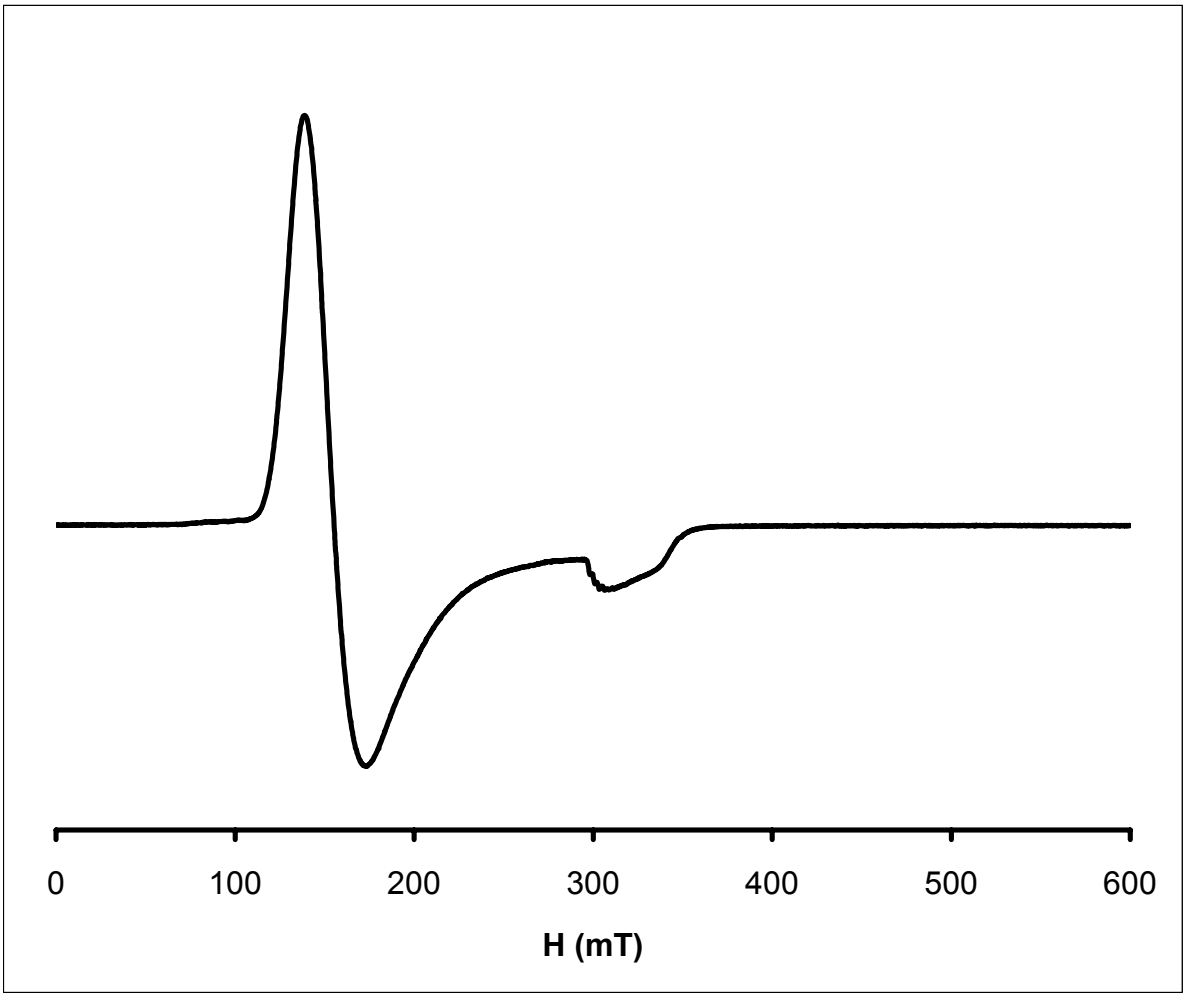
EPR spectrum of polycrystalline [$PhBP_3$]CoI (1) at 15 K.



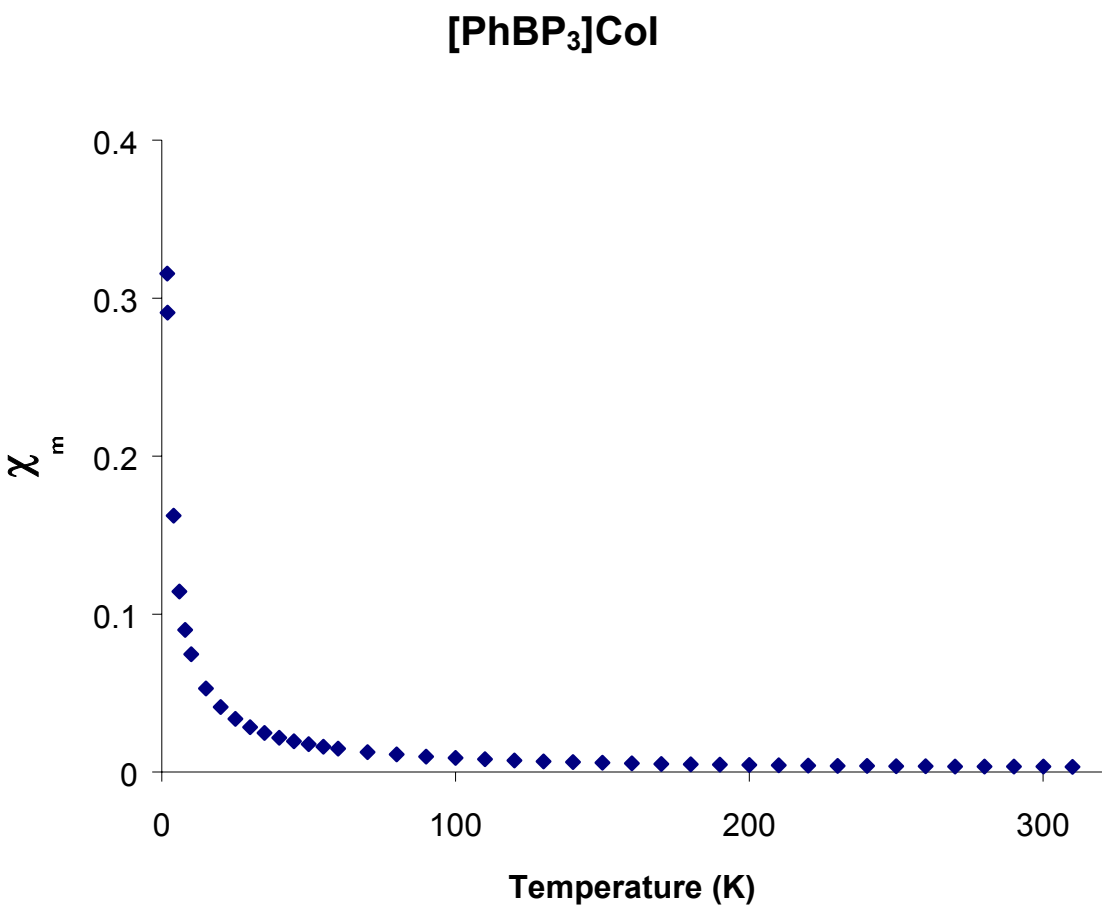
EPR spectrum of $\{[PhBP_3]Co(\mu\text{-}Br)\}_2$ (2) with admitted oxygen (toluene glass, 10 K).



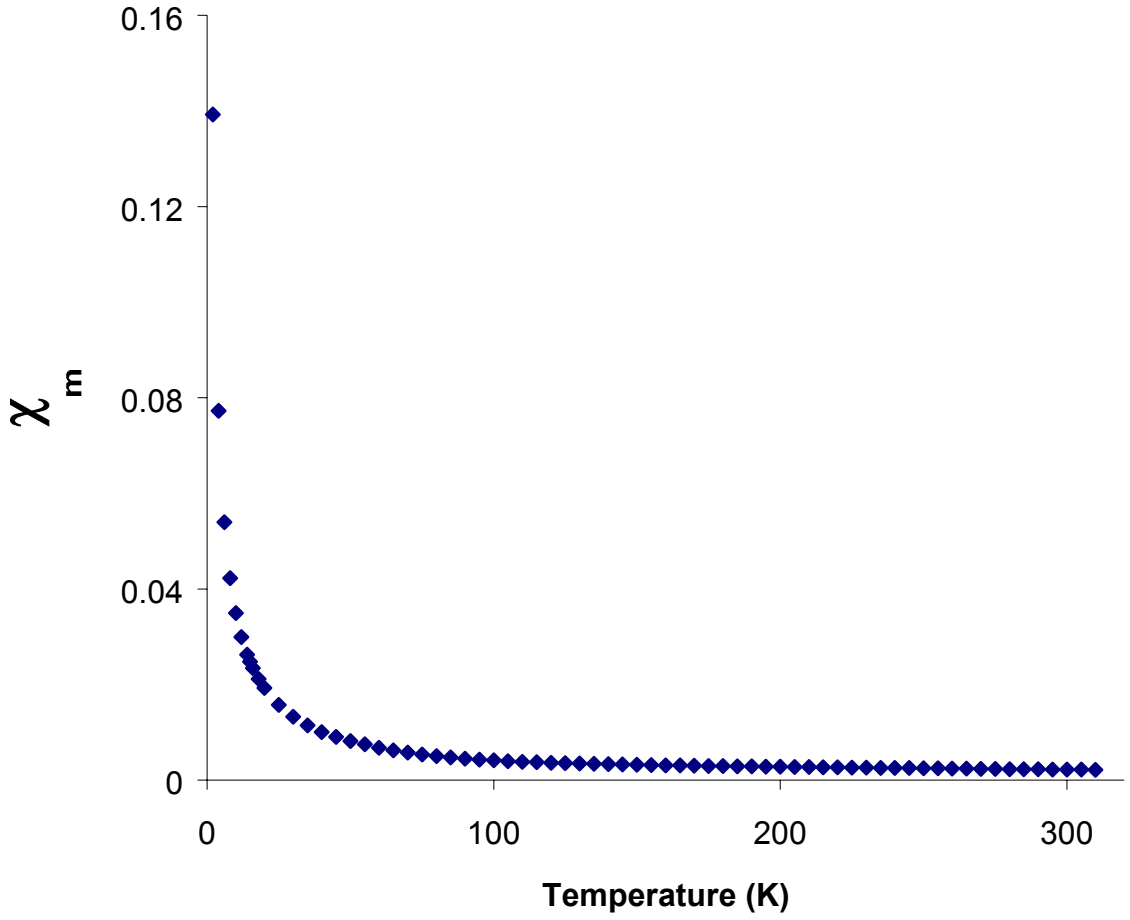
EPR spectrum of {[PhBP$_3$]Co(μ-Cl)}$_2$ (3) with admitted oxygen (toluene glass, 4 K).



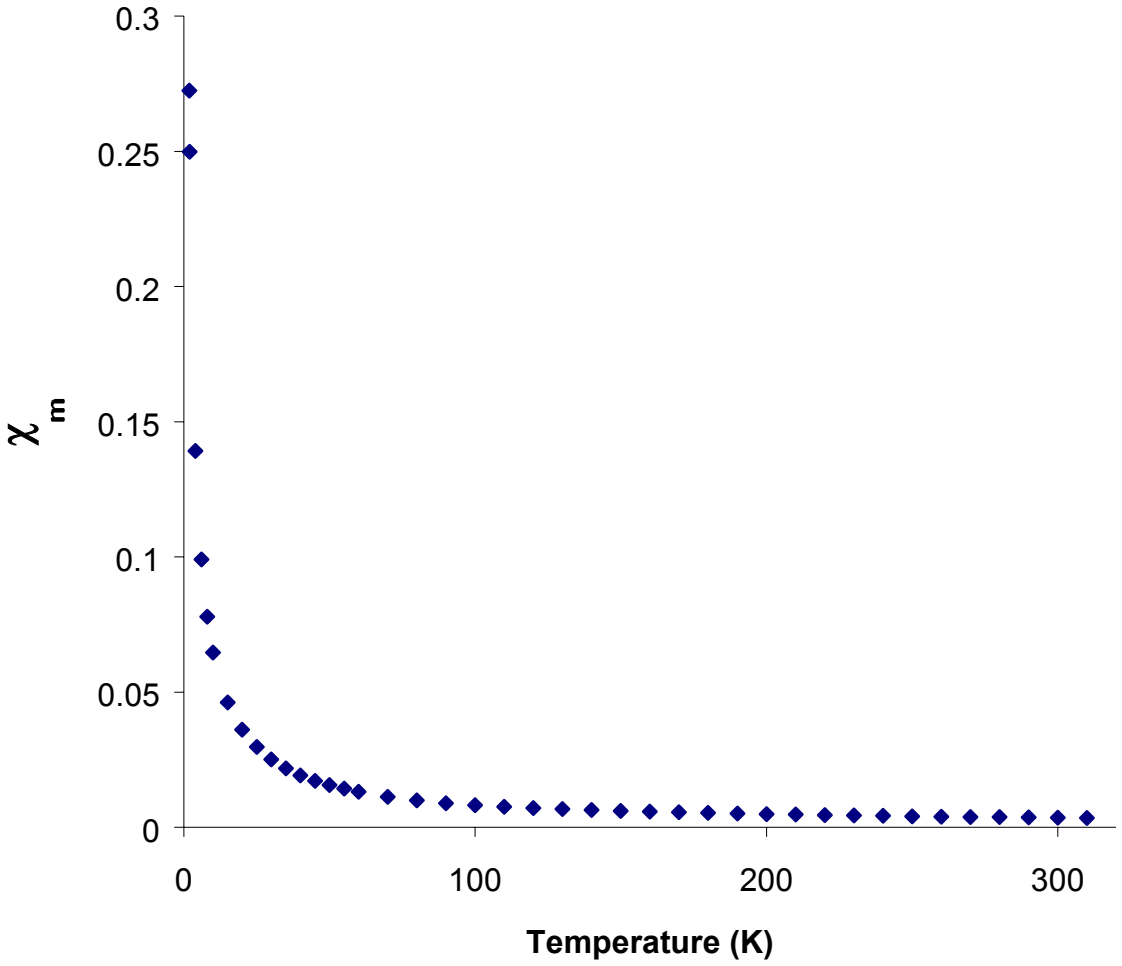
SQUID Data: χ_m versus T for [PhBP$_3$]CoI, 1.



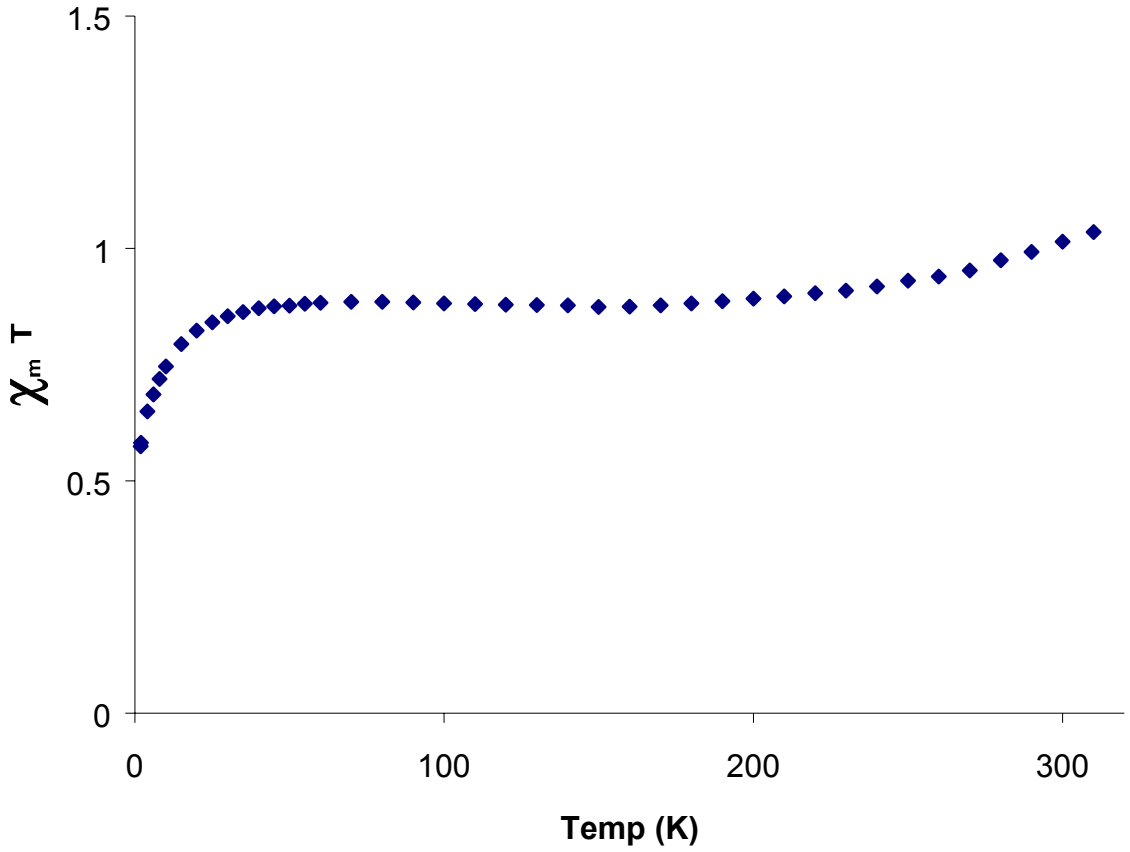
χ_m versus T for {[PhBP$_3$]Co(μ-Br)}$_2$, 2.



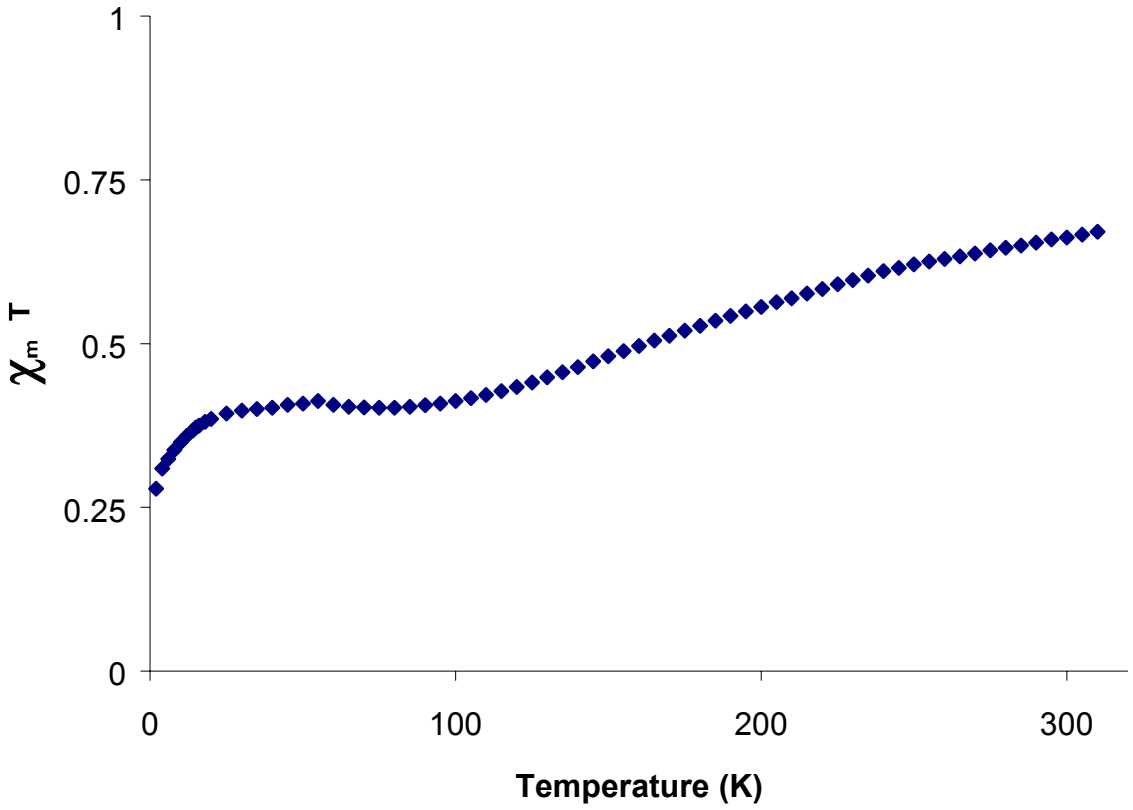
χ_m versus T for {[PhBP$_3$]Co(μ-Cl)}$_2$, 3.



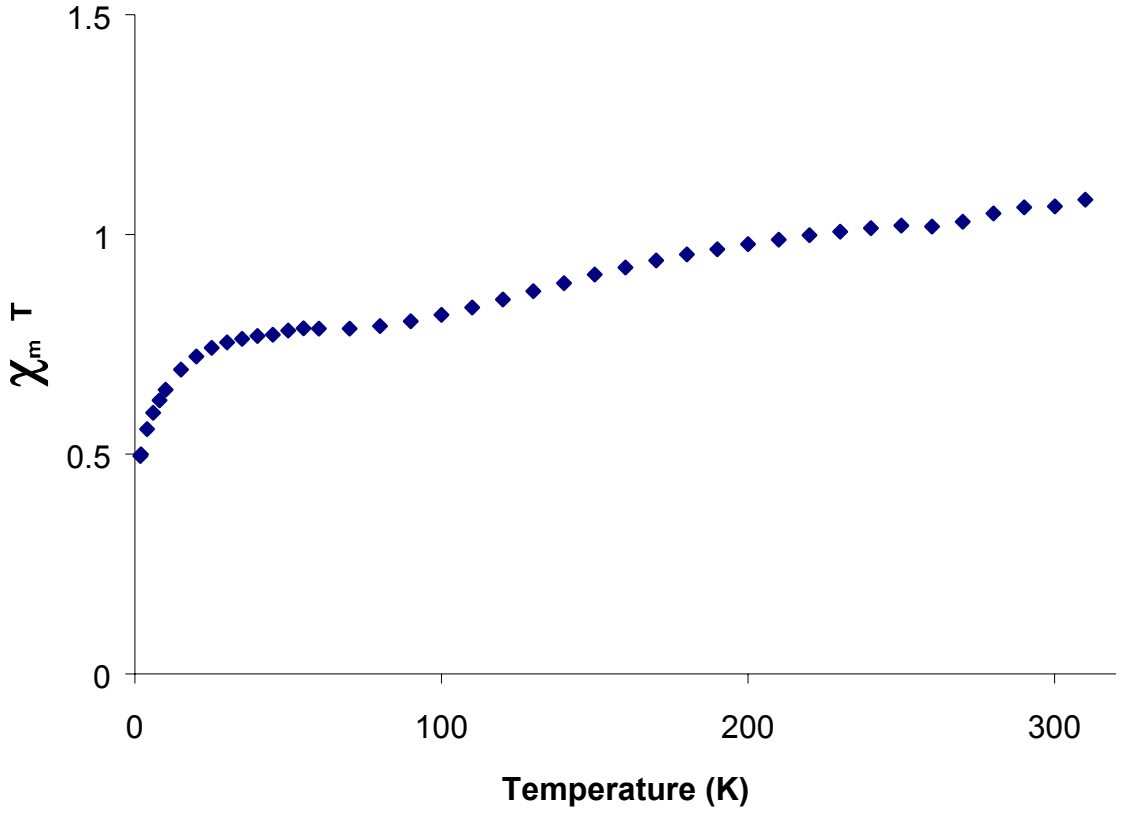
$\chi_m T$ versus T for [$PhBP_3$]CoI, 1.



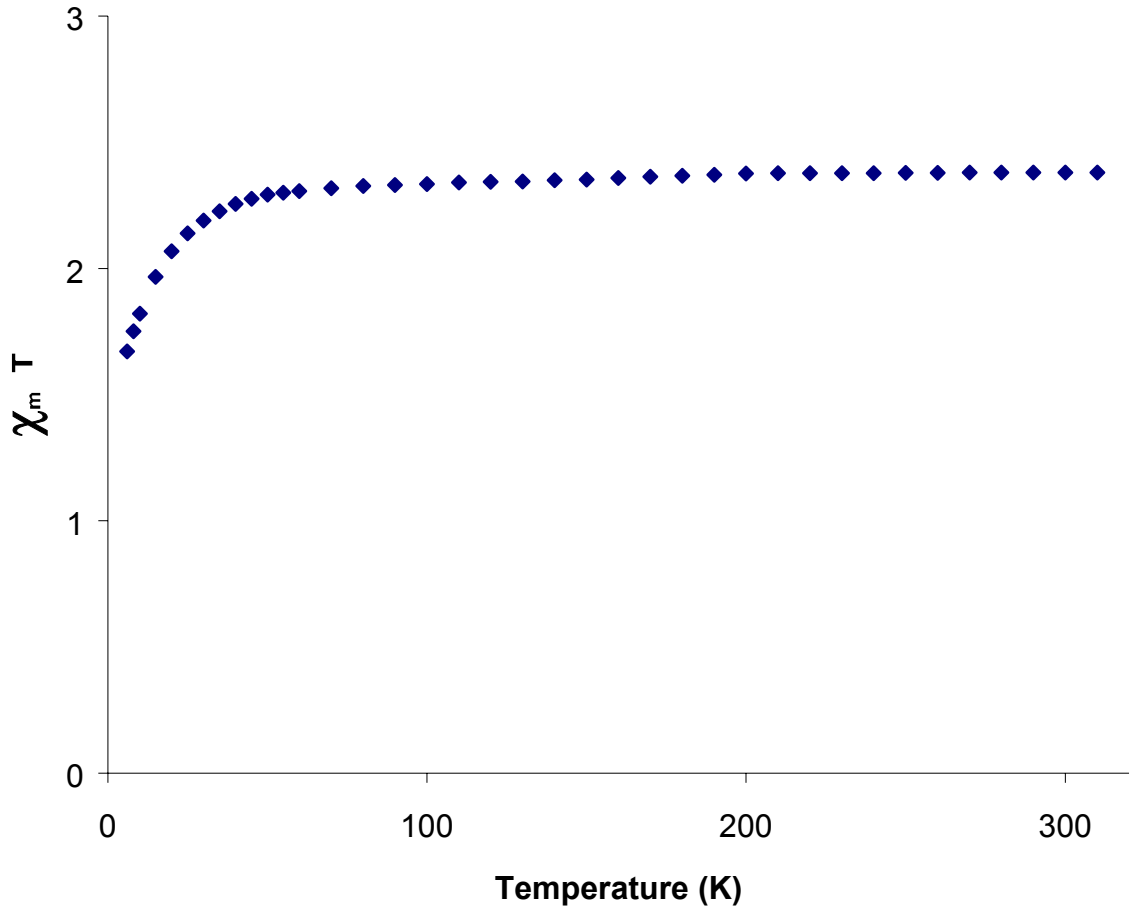
$\chi_m T$ versus T for {[PhBP$_3$]Co(μ-Br)}$_2$, 2.



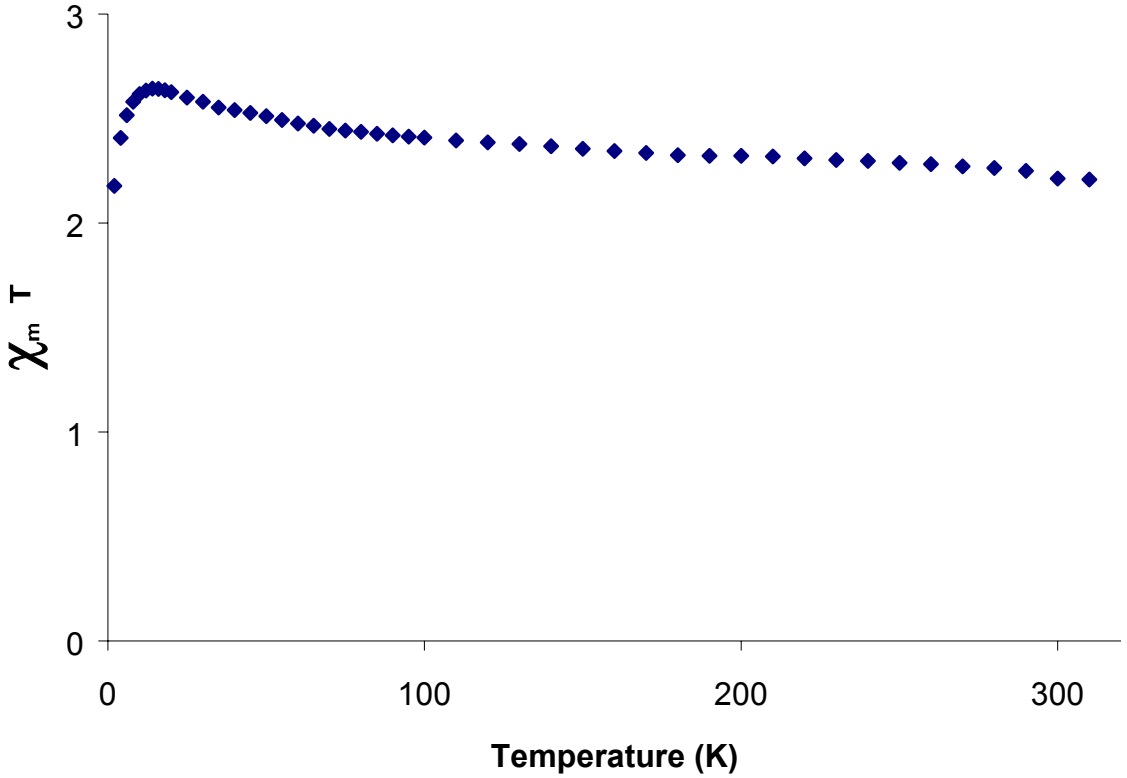
$\chi_m T$ versus T for {[PhBP$_3$]Co(μ-Cl)}$_2$, 3.



$\chi_m T$ versus T for $[PhB(CH_2PPh_2)(CH_2P(O)Ph_2)_2]CoI$, 4.



χ_mT versus T for [PhBP$_3$]Co(O-2,6-dimethylphenyl), 5.



IV.

[PhBP$_3$]CoI, 1:

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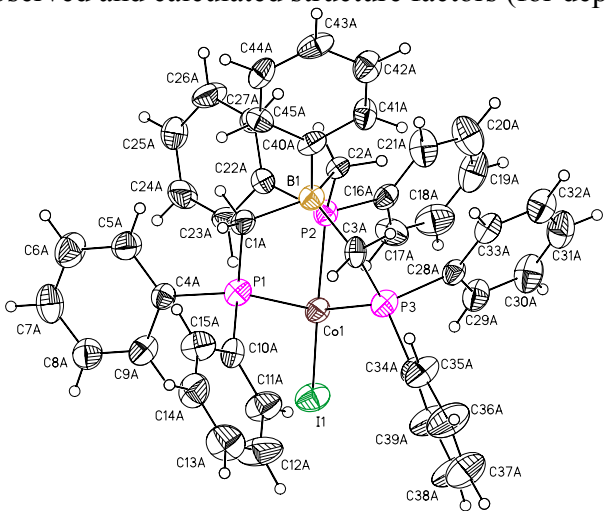


BAQ07

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 160107. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 160107."

Table 1. Crystal data and structure refinement for BAQ07 (CCDC 160107).

Empirical formula	$C_{45}H_{41}BCoIP_3 \bullet \frac{1}{2}(C_6H_6)$
Formula weight	910.38
Crystallization Solvent	Benzene
Crystal Habit	Dark green
Crystal size	0.18 x 0.13 x 0.09 mm^3
Crystal color	Blade

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 8045 reflections used in lattice determination	2.26 to 25.55°
Unit cell dimensions	a = 22.5443(17) Å b = 12.7044(9) Å β= 90.230(2)° c = 29.526(2) Å
Volume	8456.6(11) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.430 Mg/m^3
F(000)	3696
Data collection program	Bruker SMART
θ range for data collection	1.65 to 22.50°
Completeness to θ = 22.50°	100.0 %
Index ranges	$-24 \le h \le 23$, $-13 \le k \le 13$, $-31 \le l \le 31$
Data collection scan type	ω scans at 3 ϕ settings
Data reduction program	Bruker SAINT v6.2
Reflections collected	50716
Independent reflections	11064 [R_{int}= 0.1047]
Absorption coefficient	1.282 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8946 and 0.8043

Table 1 (cont.)

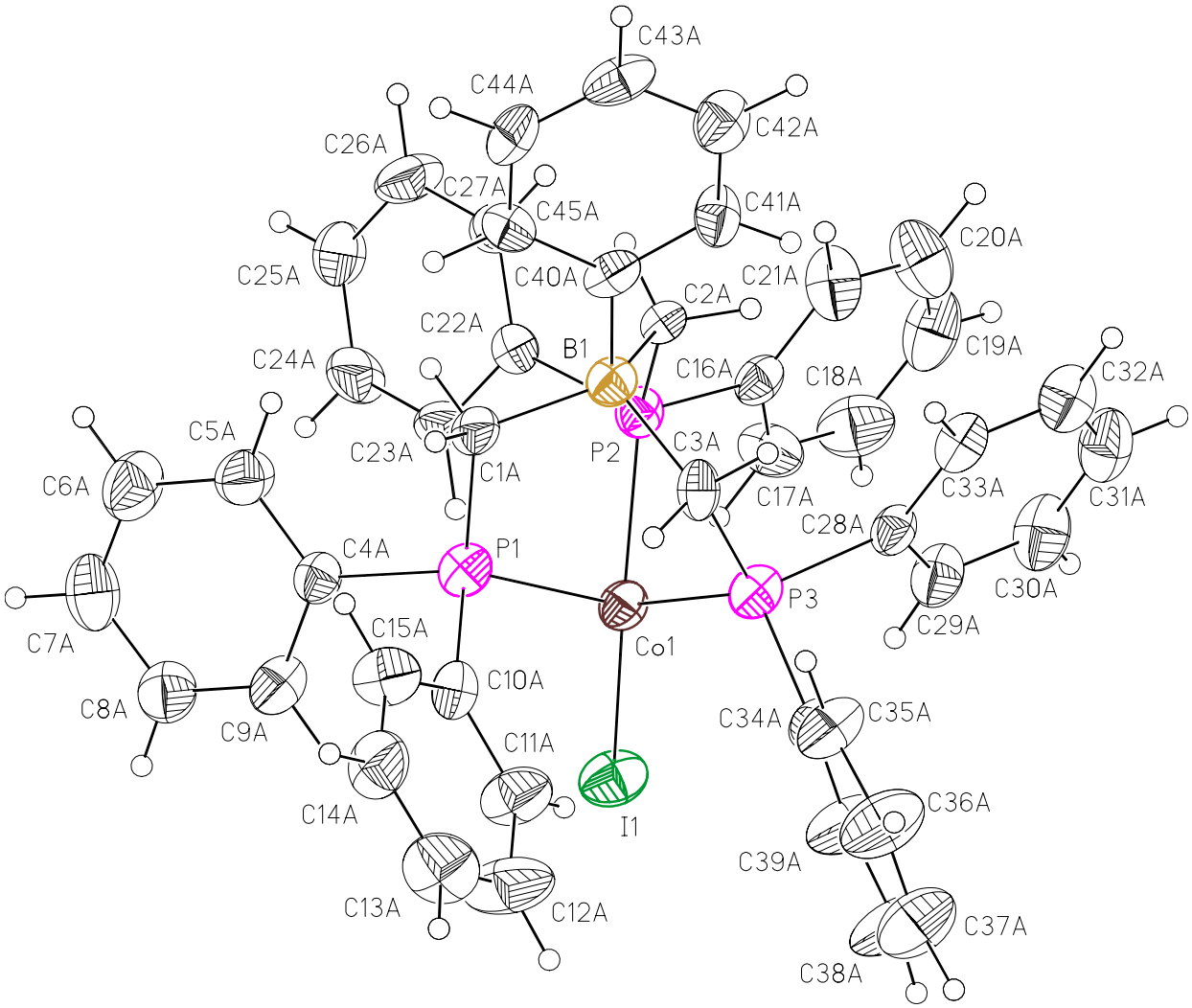
Structure solution and Refinement

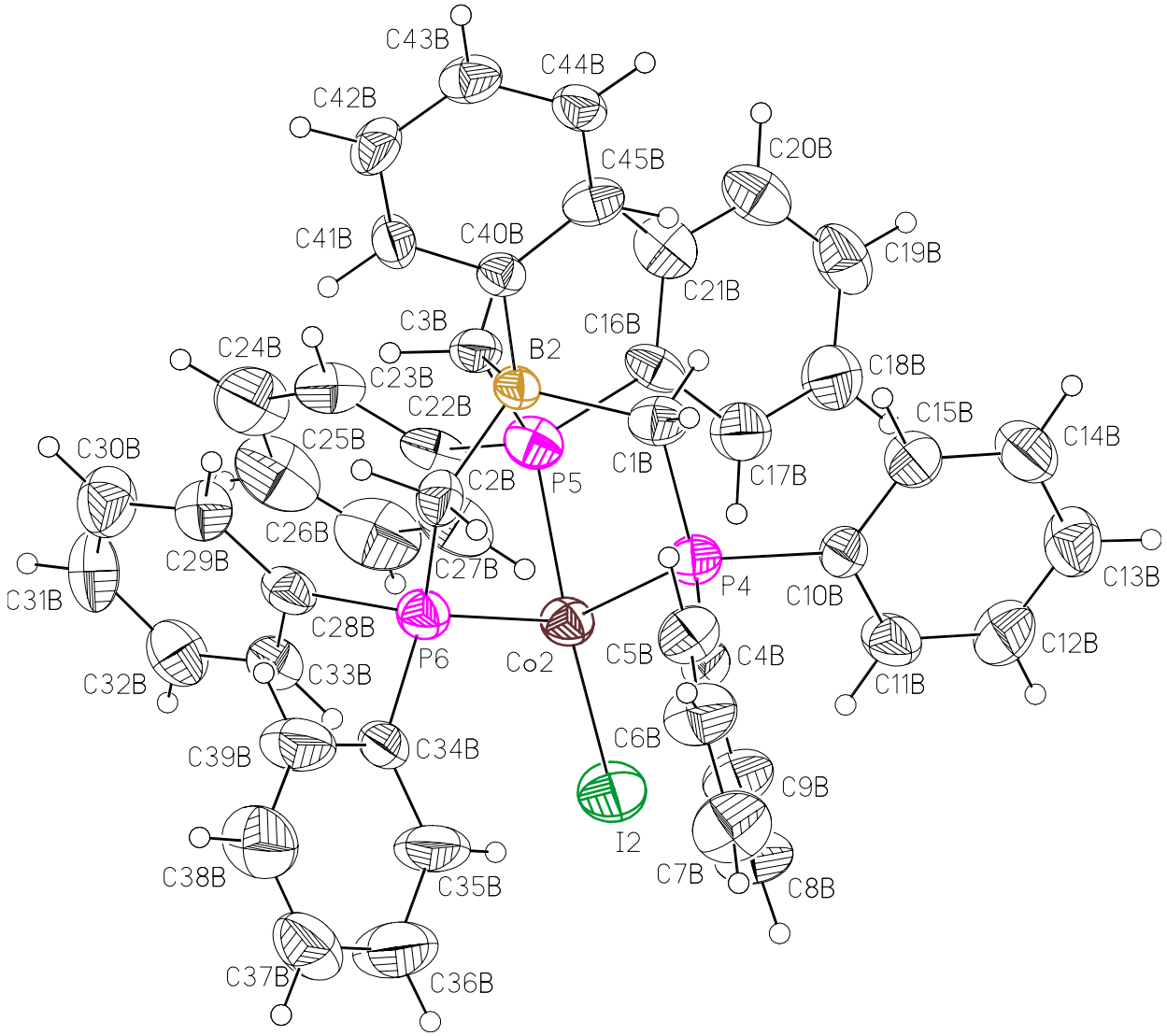
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11064 / 0 / 926
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.137
Final R indices [$I>2\sigma(I)$, 6476 reflections]	R1 = 0.0476, *w*R2 = 0.0786
R indices (all data)	R1 = 0.0899, *w*R2 = 0.0843
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.325
Average shift/error	0.004
Largest diff. peak and hole	0.775 and -0.614 e.Å^{-3}

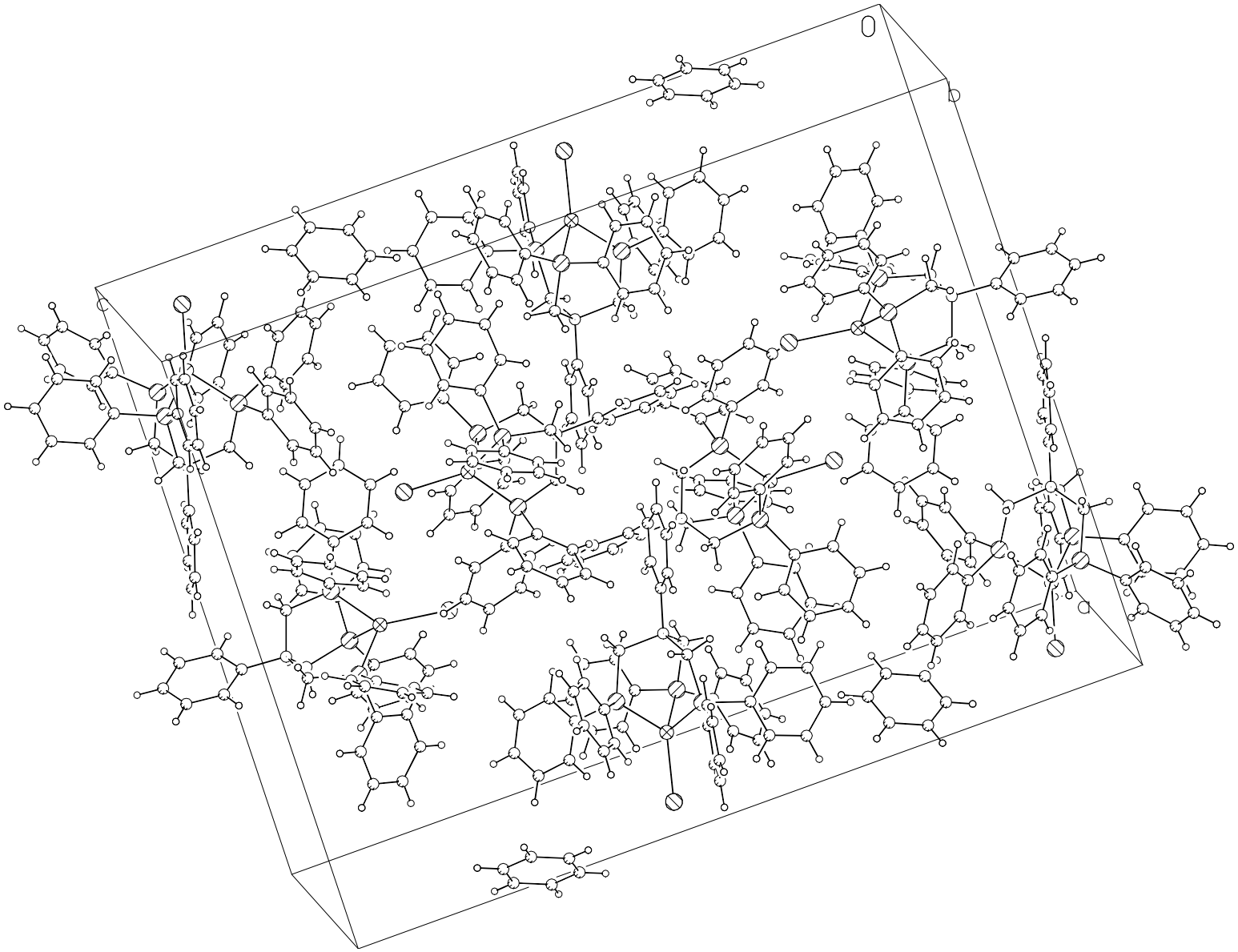
Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C43A
C44A
C42A
C26A
C27A
C45A
C41A
C20A
C25A
C40A
C21A
C2A
C22A
B1
C19A
C24A
C16A
C18A
C32A
C5A
C23A
C1A
P2
C3A
C17A
C33A
C31A
C6A
C28A
C4A
P1
P3
C30A
C7A
C15A
Co1
C29A
C10A
C8A
C9A
C34A
C35A
C11A
C14A
I1
C36A
C39A
C13A
C12A
C37A
C38A


C43B
C44B
C42B
C45B
C20B
C41B
C40B
C19B
C21B
C3B
C16B
C24B
B2
C18B
C23B
C22B
C15B
C14B
C30B
C25B
C1B
C17B
C2B
P5
C26B
C29B
C27B
C13B
C31B
P4
C10B
C28B
C12B
P6
Co2
C5B
C4B
C32B
C33B
C11B
C6B
C39B
C34B
C9B
I2
C38B
C7B
C8B
C35B
C37B
C36B



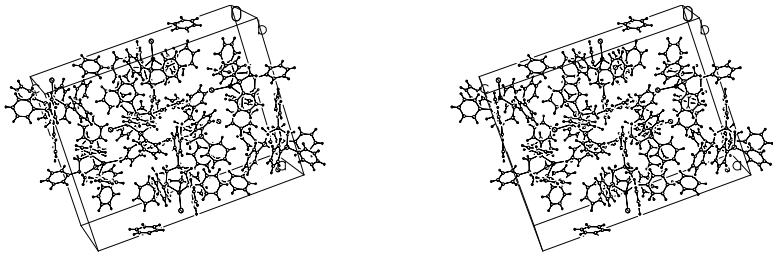


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for BAQ07 (CCDC 160107). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Co(1)	3706(1)	7351(1)	1828(1)	31(1)
I(1)	3605(1)	6965(1)	2650(1)	47(1)
P(1)	3217(1)	6339(1)	1350(1)	35(1)
P(2)	4500(1)	7265(1)	1396(1)	31(1)
P(3)	3406(1)	8885(1)	1496(1)	35(1)
B(1)	3679(3)	7751(6)	658(3)	31(2)
C(1A)	3408(3)	6580(5)	766(2)	33(2)
C(2A)	4376(3)	7790(5)	836(2)	28(2)
C(3A)	3271(3)	8679(5)	894(2)	33(2)
C(4A)	3230(3)	4918(5)	1452(2)	32(2)
C(5A)	3482(3)	4234(6)	1140(2)	47(2)
C(6A)	3480(3)	3162(6)	1222(3)	56(2)
C(7A)	3234(3)	2754(6)	1608(3)	53(2)
C(8A)	2992(3)	3443(6)	1922(2)	47(2)
C(9A)	2983(3)	4514(6)	1841(2)	42(2)
C(10A)	2429(3)	6636(5)	1408(2)	31(2)
C(11A)	2224(3)	7159(6)	1785(3)	53(2)
C(12A)	1629(4)	7385(7)	1823(3)	73(3)
C(13A)	1239(4)	7110(6)	1476(3)	63(3)
C(14A)	1439(3)	6577(6)	1109(3)	55(2)
C(15A)	2033(3)	6355(6)	1077(3)	49(2)
C(16A)	5136(3)	7937(5)	1645(2)	32(2)
C(17A)	5263(3)	7790(6)	2092(3)	48(2)
C(18A)	5758(4)	8235(7)	2293(3)	60(2)
C(19A)	6132(4)	8853(6)	2037(3)	57(2)
C(20A)	6005(4)	9013(6)	1588(3)	61(2)
C(21A)	5513(3)	8538(5)	1389(3)	47(2)
C(22A)	4823(3)	5956(5)	1345(2)	27(2)
C(23A)	4716(3)	5205(5)	1684(2)	38(2)
C(24A)	5001(3)	4243(6)	1665(3)	48(2)
C(25A)	5402(3)	4019(6)	1332(3)	50(2)
C(26A)	5515(3)	4746(6)	1001(3)	51(2)
C(27A)	5220(3)	5717(5)	1011(2)	39(2)
C(28A)	4004(3)	9825(5)	1559(2)	31(2)
C(29A)	4280(3)	9911(5)	1976(2)	44(2)
C(30A)	4738(4)	10611(6)	2046(3)	51(2)
C(31A)	4917(3)	11252(6)	1701(3)	53(2)
C(32A)	4652(3)	11215(5)	1285(3)	44(2)
C(33A)	4190(3)	10501(5)	1218(2)	36(2)
C(34A)	2793(3)	9647(5)	1716(2)	33(2)
C(35A)	2388(3)	10142(6)	1442(3)	51(2)
C(36A)	1948(4)	10789(7)	1601(3)	69(3)
C(37A)	1899(4)	10941(7)	2064(3)	71(3)
C(38A)	2281(4)	10432(7)	2350(3)	85(3)
C(39A)	2730(4)	9812(6)	2178(3)	63(3)
C(40A)	3696(3)	7977(6)	115(2)	32(2)
C(41A)	3923(3)	8910(5)	-58(2)	38(2)

C(42A)	3964(3)	9121(6)	-514(3)	44(2)
C(43A)	3773(3)	8399(6)	-830(2)	44(2)
C(44A)	3550(3)	7458(6)	-671(3)	43(2)
C(45A)	3517(3)	7250(5)	-215(2)	35(2)
Co(2)	1304(1)	1939(1)	4422(1)	36(1)
I(2)	242(1)	1716(1)	4230(1)	61(1)
P(4)	1723(1)	859(2)	4891(1)	39(1)
P(5)	2068(1)	1811(2)	3960(1)	40(1)
P(6)	1688(1)	3357(2)	4769(1)	39(1)
B(2)	2793(3)	2171(6)	4769(3)	30(2)
C(1B)	2518(3)	990(5)	4908(2)	40(2)
C(2B)	2413(3)	3124(5)	5012(2)	39(2)
C(3B)	2755(3)	2289(5)	4208(2)	35(2)
C(4B)	1435(3)	1115(5)	5453(2)	38(2)
C(5B)	1802(3)	1359(6)	5827(3)	54(2)
C(6B)	1576(4)	1524(6)	6249(3)	61(3)
C(7B)	972(4)	1429(6)	6318(3)	69(3)
C(8B)	603(4)	1149(6)	5963(3)	66(3)
C(9B)	832(3)	1021(6)	5537(3)	52(2)
C(10B)	1546(3)	-532(5)	4806(2)	36(2)
C(11B)	973(3)	-870(6)	4712(3)	52(2)
C(12B)	851(4)	-1920(7)	4662(3)	58(2)
C(13B)	1278(4)	-2661(6)	4699(3)	57(2)
C(14B)	1854(4)	-2346(6)	4779(3)	63(3)
C(15B)	1976(3)	-1289(6)	4836(2)	46(2)
C(16B)	2208(3)	516(5)	3733(2)	36(2)
C(17B)	1741(3)	-183(6)	3681(3)	51(2)
C(18B)	1826(4)	-1158(6)	3488(3)	63(3)
C(19B)	2374(4)	-1483(6)	3340(3)	57(2)
C(20B)	2842(4)	-782(7)	3389(2)	53(2)
C(21B)	2766(3)	191(6)	3582(2)	45(2)
C(22B)	1887(3)	2546(6)	3450(2)	43(2)
C(23B)	2257(3)	3333(6)	3284(3)	50(2)
C(24B)	2086(4)	3926(7)	2904(3)	70(3)
C(25B)	1561(5)	3723(8)	2694(3)	75(3)
C(26B)	1196(4)	2960(8)	2848(3)	77(3)
C(27B)	1352(4)	2378(6)	3230(3)	58(2)
C(28B)	1753(3)	4383(5)	4335(2)	39(2)
C(29B)	2242(3)	5009(6)	4259(3)	45(2)
C(30B)	2230(4)	5749(6)	3917(3)	61(3)
C(31B)	1738(4)	5875(6)	3650(3)	63(3)
C(32B)	1241(4)	5267(6)	3726(3)	54(2)
C(33B)	1245(3)	4522(6)	4064(3)	47(2)
C(34B)	1242(3)	4055(6)	5177(3)	40(2)
C(35B)	678(4)	3803(6)	5272(3)	78(3)
C(36B)	321(4)	4388(8)	5553(3)	94(4)
C(37B)	552(4)	5252(7)	5767(3)	69(3)
C(38B)	1128(4)	5504(7)	5691(3)	75(3)
C(39B)	1461(4)	4915(7)	5408(3)	64(3)
C(40B)	3491(3)	2200(5)	4916(2)	30(2)
C(41B)	3808(3)	3133(5)	4942(2)	40(2)
C(42B)	4399(3)	3196(6)	5063(2)	44(2)
C(43B)	4703(3)	2280(6)	5174(2)	43(2)
C(44B)	4406(3)	1325(6)	5143(2)	39(2)

C(45B)	3817(3)	1288(6)	5007(2)	40(2)
C(101)	348(6)	441(15)	1972(3)	284(4)
C(102)	-41(7)	1255(10)	2075(5)	284(4)
C(103)	-285(4)	1325(8)	2505(7)	284(4)
C(104)	-141(6)	581(15)	2832(3)	284(4)
C(105)	248(6)	-233(10)	2730(5)	284(4)
C(106)	493(4)	-303(9)	2299(7)	284(4)

Table 3. Selected bond lengths [Å] and angles [°] for BAQ07 (CCDC 160107).

Co(1)-P(1)	2.200(2)	P(1)-Co(1)-P(2)	90.33(8)
Co(1)-P(2)	2.206(2)	P(1)-Co(1)-P(3)	94.46(7)
Co(1)-P(3)	2.282(2)	P(2)-Co(1)-P(3)	91.95(7)
Co(1)-I(1)	2.4883(10)	P(1)-Co(1)-I(1)	117.54(6)
Co(2)-P(4)	2.163(2)	P(2)-Co(1)-I(1)	129.19(6)
Co(2)-P(5)	2.208(2)	P(3)-Co(1)-I(1)	124.01(6)
Co(2)-P(6)	2.244(2)	P(4)-Co(2)-P(5)	90.53(8)
Co(2)-I(2)	2.4739(10)	P(4)-Co(2)-P(6)	92.89(8)
		P(5)-Co(2)-P(6)	92.31(8)
		P(4)-Co(2)-I(2)	119.59(7)
		P(5)-Co(2)-I(2)	127.33(6)
		P(6)-Co(2)-I(2)	124.59(6)

Table 4. Bond lengths [Å] and angles [°] for BAQ07 (CCDC 160107).

Co(1)-P(1)	2.200(2)	C(19A)-C(20A)	1.371(9)
Co(1)-P(2)	2.206(2)	C(19A)-H(19A)	0.9500
Co(1)-P(3)	2.282(2)	C(20A)-C(21A)	1.392(9)
Co(1)-I(1)	2.4883(10)	C(20A)-H(20A)	0.9500
P(1)-C(10A)	1.826(7)	C(21A)-H(21A)	0.9500
P(1)-C(4A)	1.830(6)	C(22A)-C(27A)	1.367(8)
P(1)-C(1A)	1.806(6)	C(22A)-C(23A)	1.405(8)
P(2)-C(22A)	1.821(6)	C(23A)-C(24A)	1.383(8)
P(2)-C(2A)	1.804(6)	C(23A)-H(23A)	0.9500
P(2)-C(16A)	1.822(7)	C(24A)-C(25A)	1.368(9)
P(3)-C(34A)	1.811(7)	C(24A)-H(24A)	0.9500
P(3)-C(28A)	1.811(7)	C(25A)-C(26A)	1.370(9)
P(3)-C(3A)	1.819(6)	C(25A)-H(25A)	0.9500
B(1)-C(40A)	1.630(9)	C(26A)-C(27A)	1.401(8)
B(1)-C(2A)	1.655(9)	C(26A)-H(26A)	0.9500
B(1)-C(1A)	1.639(9)	C(27A)-H(27A)	0.9500
B(1)-C(3A)	1.652(9)	C(28A)-C(29A)	1.381(8)
C(1A)-H(1A1)	0.9900	C(28A)-C(33A)	1.388(8)
C(1A)-H(1A2)	0.9900	C(29A)-C(30A)	1.378(9)
C(2A)-H(2A1)	0.9900	C(29A)-H(29A)	0.9500
C(2A)-H(2A2)	0.9900	C(30A)-C(31A)	1.366(9)
C(3A)-H(3A1)	0.9900	C(30A)-H(30A)	0.9500
C(3A)-H(3A2)	0.9900	C(31A)-C(32A)	1.366(9)
C(4A)-C(5A)	1.388(8)	C(31A)-H(31A)	0.9500
C(4A)-C(9A)	1.380(8)	C(32A)-C(33A)	1.395(8)
C(5A)-C(6A)	1.383(9)	C(32A)-H(32A)	0.9500
C(5A)-H(5A)	0.9500	C(33A)-H(33A)	0.9500
C(6A)-C(7A)	1.371(9)	C(34A)-C(35A)	1.370(8)
C(6A)-H(6A)	0.9500	C(34A)-C(39A)	1.390(9)
C(7A)-C(8A)	1.388(9)	C(35A)-C(36A)	1.374(9)
C(7A)-H(7A)	0.9500	C(35A)-H(35A)	0.9500
C(8A)-C(9A)	1.381(8)	C(36A)-C(37A)	1.386(10)
C(8A)-H(8A)	0.9500	C(36A)-H(36A)	0.9500
C(9A)-H(9A)	0.9500	C(37A)-C(38A)	1.367(10)
C(10A)-C(15A)	1.368(8)	C(37A)-H(37A)	0.9500
C(10A)-C(11A)	1.380(8)	C(38A)-C(39A)	1.381(9)
C(11A)-C(12A)	1.377(9)	C(38A)-H(38A)	0.9500
C(11A)-H(11A)	0.9500	C(39A)-H(39A)	0.9500
C(12A)-C(13A)	1.392(10)	C(40A)-C(41A)	1.390(8)
C(12A)-H(12A)	0.9500	C(40A)-C(45A)	1.402(8)
C(13A)-C(14A)	1.358(9)	C(41A)-C(42A)	1.378(8)
C(13A)-H(13A)	0.9500	C(41A)-H(41A)	0.9500
C(14A)-C(15A)	1.370(9)	C(42A)-C(43A)	1.375(8)
C(14A)-H(14A)	0.9500	C(42A)-H(42A)	0.9500
C(15A)-H(15A)	0.9500	C(43A)-C(44A)	1.381(9)
C(16A)-C(17A)	1.364(8)	C(43A)-H(43A)	0.9500
C(16A)-C(21A)	1.371(8)	C(44A)-C(45A)	1.373(9)
C(17A)-C(18A)	1.383(9)	C(44A)-H(44A)	0.9500
C(17A)-H(17A)	0.9500	C(45A)-H(45A)	0.9500
C(18A)-C(19A)	1.380(10)	Co(2)-P(4)	2.163(2)
C(18A)-H(18A)	0.9500	Co(2)-P(5)	2.208(2)

Co(2)-P(6)	2.244(2)	C(22B)-C(23B)	1.391(9)
Co(2)-I(2)	2.4739(10)	C(22B)-C(27B)	1.384(9)
P(4)-C(4B)	1.811(7)	C(23B)-C(24B)	1.405(9)
P(4)-C(10B)	1.829(7)	C(23B)-H(23B)	0.9500
P(4)-C(1B)	1.801(6)	C(24B)-C(25B)	1.360(11)
P(5)-C(16B)	1.805(7)	C(24B)-H(24B)	0.9500
P(5)-C(22B)	1.817(7)	C(25B)-C(26B)	1.351(11)
P(5)-C(3B)	1.814(6)	C(25B)-H(25B)	0.9500
P(6)-C(28B)	1.834(7)	C(26B)-C(27B)	1.394(10)
P(6)-C(34B)	1.805(7)	C(26B)-H(26B)	0.9500
P(6)-C(2B)	1.808(6)	C(27B)-H(27B)	0.9500
B(2)-C(40B)	1.631(9)	C(28B)-C(33B)	1.405(8)
B(2)-C(2B)	1.648(9)	C(28B)-C(29B)	1.378(9)
B(2)-C(3B)	1.665(9)	C(29B)-C(30B)	1.380(9)
B(2)-C(1B)	1.674(9)	C(29B)-H(29B)	0.9500
C(1B)-H(1B1)	0.9900	C(30B)-C(31B)	1.368(9)
C(1B)-H(1B2)	0.9900	C(30B)-H(30B)	0.9500
C(2B)-H(2B1)	0.9900	C(31B)-C(32B)	1.380(9)
C(2B)-H(2B2)	0.9900	C(31B)-H(31B)	0.9500
C(3B)-H(3B1)	0.9900	C(32B)-C(33B)	1.377(9)
C(3B)-H(3B2)	0.9900	C(32B)-H(32B)	0.9500
C(4B)-C(5B)	1.413(9)	C(33B)-H(33B)	0.9500
C(4B)-C(9B)	1.388(9)	C(34B)-C(35B)	1.343(9)
C(5B)-C(6B)	1.365(9)	C(34B)-C(39B)	1.378(9)
C(5B)-H(5B)	0.9500	C(35B)-C(36B)	1.376(10)
C(6B)-C(7B)	1.382(10)	C(35B)-H(35B)	0.9500
C(6B)-H(6B)	0.9500	C(36B)-C(37B)	1.369(10)
C(7B)-C(8B)	1.384(10)	C(36B)-H(36B)	0.9500
C(7B)-H(7B)	0.9500	C(37B)-C(38B)	1.356(10)
C(8B)-C(9B)	1.370(9)	C(37B)-H(37B)	0.9500
C(8B)-H(8B)	0.9500	C(38B)-C(39B)	1.351(10)
C(9B)-H(9B)	0.9500	C(38B)-H(38B)	0.9500
C(10B)-C(15B)	1.367(8)	C(39B)-H(39B)	0.9500
C(10B)-C(11B)	1.390(9)	C(40B)-C(41B)	1.387(8)
C(11B)-C(12B)	1.370(9)	C(40B)-C(45B)	1.396(8)
C(11B)-H(11B)	0.9500	C(41B)-C(42B)	1.378(8)
C(12B)-C(13B)	1.350(9)	C(41B)-H(41B)	0.9500
C(12B)-H(12B)	0.9500	C(42B)-C(43B)	1.390(8)
C(13B)-C(14B)	1.380(9)	C(42B)-H(42B)	0.9500
C(13B)-H(13B)	0.9500	C(43B)-C(44B)	1.388(8)
C(14B)-C(15B)	1.381(9)	C(43B)-H(43B)	0.9500
C(14B)-H(14B)	0.9500	C(44B)-C(45B)	1.388(8)
C(15B)-H(15B)	0.9500	C(44B)-H(44B)	0.9500
C(16B)-C(21B)	1.399(9)	C(45B)-H(45B)	0.9500
C(16B)-C(17B)	1.385(9)	C(101)-C(102)	1.3900
C(17B)-C(18B)	1.378(9)	C(101)-C(106)	1.3900
C(17B)-H(17B)	0.9500	C(101)-H(101)	0.9500
C(18B)-C(19B)	1.375(9)	C(102)-C(103)	1.3900
C(18B)-H(18B)	0.9500	C(102)-H(102)	0.9500
C(19B)-C(20B)	1.387(9)	C(103)-C(104)	1.3900
C(19B)-H(19B)	0.9500	C(103)-H(103)	0.9500
C(20B)-C(21B)	1.374(9)	C(104)-C(105)	1.3900
C(20B)-H(20B)	0.9500	C(104)-H(104)	0.9500
C(21B)-H(21B)	0.9500	C(105)-C(106)	1.3900

C(105)-H(105)	0.9500	C(6A)-C(5A)-C(4A)	119.9(7)
C(106)-H(106)	0.9500	C(6A)-C(5A)-H(5A)	120.1
		C(4A)-C(5A)-H(5A)	120.1
P(1)-Co(1)-P(2)	90.33(8)	C(7A)-C(6A)-C(5A)	121.3(8)
P(1)-Co(1)-P(3)	94.46(7)	C(7A)-C(6A)-H(6A)	119.3
P(2)-Co(1)-P(3)	91.95(7)	C(5A)-C(6A)-H(6A)	119.3
P(1)-Co(1)-I(1)	117.54(6)	C(6A)-C(7A)-C(8A)	118.5(7)
P(2)-Co(1)-I(1)	129.19(6)	C(6A)-C(7A)-H(7A)	120.7
P(3)-Co(1)-I(1)	124.01(6)	C(8A)-C(7A)-H(7A)	120.7
C(10A)-P(1)-C(4A)	101.8(3)	C(7A)-C(8A)-C(9A)	120.7(7)
C(10A)-P(1)-C(1A)	106.8(3)	C(7A)-C(8A)-H(8A)	119.6
C(4A)-P(1)-C(1A)	108.7(3)	C(9A)-C(8A)-H(8A)	119.6
C(10A)-P(1)-Co(1)	107.7(2)	C(8A)-C(9A)-C(4A)	120.3(7)
C(4A)-P(1)-Co(1)	117.7(2)	C(8A)-C(9A)-H(9A)	119.8
C(1A)-P(1)-Co(1)	113.1(2)	C(4A)-C(9A)-H(9A)	119.8
C(22A)-P(2)-C(2A)	108.8(3)	C(15A)-C(10A)-C(11A)	118.9(7)
C(22A)-P(2)-C(16A)	98.5(3)	C(15A)-C(10A)-P(1)	120.9(6)
C(2A)-P(2)-C(16A)	108.4(3)	C(11A)-C(10A)-P(1)	120.2(5)
C(22A)-P(2)-Co(1)	114.8(2)	C(12A)-C(11A)-C(10A)	119.7(7)
C(2A)-P(2)-Co(1)	112.8(2)	C(12A)-C(11A)-H(11A)	120.2
C(16A)-P(2)-Co(1)	112.5(2)	C(10A)-C(11A)-H(11A)	120.2
C(34A)-P(3)-C(28A)	100.4(3)	C(11A)-C(12A)-C(13A)	120.1(8)
C(34A)-P(3)-C(3A)	107.6(3)	C(11A)-C(12A)-H(12A)	119.9
C(28A)-P(3)-C(3A)	108.4(3)	C(13A)-C(12A)-H(12A)	119.9
C(34A)-P(3)-Co(1)	121.8(2)	C(14A)-C(13A)-C(12A)	120.1(8)
C(28A)-P(3)-Co(1)	107.5(2)	C(14A)-C(13A)-H(13A)	120.0
C(3A)-P(3)-Co(1)	110.2(2)	C(12A)-C(13A)-H(13A)	120.0
C(40A)-B(1)-C(2A)	106.2(5)	C(13A)-C(14A)-C(15A)	119.0(8)
C(40A)-B(1)-C(1A)	111.2(6)	C(13A)-C(14A)-H(14A)	120.5
C(2A)-B(1)-C(1A)	108.6(5)	C(15A)-C(14A)-H(14A)	120.5
C(40A)-B(1)-C(3A)	107.7(5)	C(10A)-C(15A)-C(14A)	122.2(7)
C(2A)-B(1)-C(3A)	112.0(5)	C(10A)-C(15A)-H(15A)	118.9
C(1A)-B(1)-C(3A)	111.0(5)	C(14A)-C(15A)-H(15A)	118.9
B(1)-C(1A)-P(1)	115.4(4)	C(17A)-C(16A)-C(21A)	118.9(7)
B(1)-C(1A)-H(1A1)	108.4	C(17A)-C(16A)-P(2)	119.2(6)
P(1)-C(1A)-H(1A1)	108.4	C(21A)-C(16A)-P(2)	121.7(6)
B(1)-C(1A)-H(1A2)	108.4	C(16A)-C(17A)-C(18A)	121.6(7)
P(1)-C(1A)-H(1A2)	108.4	C(16A)-C(17A)-H(17A)	119.2
H(1A1)-C(1A)-H(1A2)	107.5	C(18A)-C(17A)-H(17A)	119.2
B(1)-C(2A)-P(2)	115.0(4)	C(17A)-C(18A)-C(19A)	119.4(8)
B(1)-C(2A)-H(2A1)	108.5	C(17A)-C(18A)-H(18A)	120.3
P(2)-C(2A)-H(2A1)	108.5	C(19A)-C(18A)-H(18A)	120.3
B(1)-C(2A)-H(2A2)	108.5	C(20A)-C(19A)-C(18A)	119.3(8)
P(2)-C(2A)-H(2A2)	108.5	C(20A)-C(19A)-H(19A)	120.3
H(2A1)-C(2A)-H(2A2)	107.5	C(18A)-C(19A)-H(19A)	120.3
B(1)-C(3A)-P(3)	115.0(4)	C(19A)-C(20A)-C(21A)	120.5(8)
B(1)-C(3A)-H(3A1)	108.5	C(19A)-C(20A)-H(20A)	119.8
P(3)-C(3A)-H(3A1)	108.5	C(21A)-C(20A)-H(20A)	119.8
B(1)-C(3A)-H(3A2)	108.5	C(16A)-C(21A)-C(20A)	120.2(7)
P(3)-C(3A)-H(3A2)	108.5	C(16A)-C(21A)-H(21A)	119.9
H(3A1)-C(3A)-H(3A2)	107.5	C(20A)-C(21A)-H(21A)	119.9
C(5A)-C(4A)-C(9A)	119.2(6)	C(27A)-C(22A)-C(23A)	118.5(6)
C(5A)-C(4A)-P(1)	121.0(6)	C(27A)-C(22A)-P(2)	121.7(5)
C(9A)-C(4A)-P(1)	119.8(6)	C(23A)-C(22A)-P(2)	119.4(5)

C(24A)-C(23A)-C(22A)	119.3(7)	C(42A)-C(41A)-C(40A)	123.5(7)
C(24A)-C(23A)-H(23A)	120.3	C(42A)-C(41A)-H(41A)	118.3
C(22A)-C(23A)-H(23A)	120.3	C(40A)-C(41A)-H(41A)	118.3
C(23A)-C(24A)-C(25A)	121.4(7)	C(41A)-C(42A)-C(43A)	120.7(7)
C(23A)-C(24A)-H(24A)	119.3	C(41A)-C(42A)-H(42A)	119.6
C(25A)-C(24A)-H(24A)	119.3	C(43A)-C(42A)-H(42A)	119.6
C(26A)-C(25A)-C(24A)	119.9(7)	C(44A)-C(43A)-C(42A)	117.4(7)
C(26A)-C(25A)-H(25A)	120.1	C(44A)-C(43A)-H(43A)	121.3
C(24A)-C(25A)-H(25A)	120.1	C(42A)-C(43A)-H(43A)	121.3
C(27A)-C(26A)-C(25A)	119.2(7)	C(45A)-C(44A)-C(43A)	121.5(7)
C(27A)-C(26A)-H(26A)	120.4	C(45A)-C(44A)-H(44A)	119.3
C(25A)-C(26A)-H(26A)	120.4	C(43A)-C(44A)-H(44A)	119.3
C(22A)-C(27A)-C(26A)	121.5(7)	C(44A)-C(45A)-C(40A)	122.5(7)
C(22A)-C(27A)-H(27A)	119.2	C(44A)-C(45A)-H(45A)	118.7
C(26A)-C(27A)-H(27A)	119.2	C(40A)-C(45A)-H(45A)	118.7
C(29A)-C(28A)-C(33A)	117.5(6)	P(4)-Co(2)-P(5)	90.53(8)
C(29A)-C(28A)-P(3)	118.4(6)	P(4)-Co(2)-P(6)	92.89(8)
C(33A)-C(28A)-P(3)	124.1(6)	P(5)-Co(2)-P(6)	92.31(8)
C(30A)-C(29A)-C(28A)	121.3(7)	P(4)-Co(2)-I(2)	119.59(7)
C(30A)-C(29A)-H(29A)	119.3	P(5)-Co(2)-I(2)	127.33(6)
C(28A)-C(29A)-H(29A)	119.3	P(6)-Co(2)-I(2)	124.59(6)
C(29A)-C(30A)-C(31A)	119.7(7)	C(4B)-P(4)-C(10B)	102.8(3)
C(29A)-C(30A)-H(30A)	120.1	C(4B)-P(4)-C(1B)	108.6(3)
C(31A)-C(30A)-H(30A)	120.1	C(10B)-P(4)-C(1B)	108.0(3)
C(30A)-C(31A)-C(32A)	121.4(8)	C(4B)-P(4)-Co(2)	108.4(2)
C(30A)-C(31A)-H(31A)	119.3	C(10B)-P(4)-Co(2)	115.5(2)
C(32A)-C(31A)-H(31A)	119.3	C(1B)-P(4)-Co(2)	113.0(2)
C(33A)-C(32A)-C(31A)	118.3(7)	C(16B)-P(5)-C(22B)	101.5(3)
C(33A)-C(32A)-H(32A)	120.9	C(16B)-P(5)-C(3B)	107.8(3)
C(31A)-C(32A)-H(32A)	120.9	C(22B)-P(5)-C(3B)	110.5(3)
C(32A)-C(33A)-C(28A)	121.8(7)	C(16B)-P(5)-Co(2)	115.8(3)
C(32A)-C(33A)-H(33A)	119.1	C(22B)-P(5)-Co(2)	107.5(2)
C(28A)-C(33A)-H(33A)	119.1	C(3B)-P(5)-Co(2)	113.1(2)
C(35A)-C(34A)-C(39A)	116.2(7)	C(28B)-P(6)-C(34B)	99.4(3)
C(35A)-C(34A)-P(3)	122.7(6)	C(28B)-P(6)-C(2B)	108.6(3)
C(39A)-C(34A)-P(3)	120.9(6)	C(34B)-P(6)-C(2B)	108.7(3)
C(34A)-C(35A)-C(36A)	123.5(8)	C(28B)-P(6)-Co(2)	106.5(2)
C(34A)-C(35A)-H(35A)	118.2	C(34B)-P(6)-Co(2)	119.0(3)
C(36A)-C(35A)-H(35A)	118.2	C(2B)-P(6)-Co(2)	113.3(2)
C(37A)-C(36A)-C(35A)	118.8(8)	C(40B)-B(2)-C(2B)	111.7(5)
C(37A)-C(36A)-H(36A)	120.6	C(40B)-B(2)-C(3B)	107.9(5)
C(35A)-C(36A)-H(36A)	120.6	C(2B)-B(2)-C(3B)	110.0(5)
C(38A)-C(37A)-C(36A)	119.4(8)	C(40B)-B(2)-C(1B)	108.2(5)
C(38A)-C(37A)-H(37A)	120.3	C(2B)-B(2)-C(1B)	111.1(5)
C(36A)-C(37A)-H(37A)	120.3	C(3B)-B(2)-C(1B)	107.8(5)
C(37A)-C(38A)-C(39A)	120.3(9)	B(2)-C(1B)-P(4)	116.4(4)
C(37A)-C(38A)-H(38A)	119.9	B(2)-C(1B)-H(1B1)	108.2
C(39A)-C(38A)-H(38A)	119.9	P(4)-C(1B)-H(1B1)	108.2
C(34A)-C(39A)-C(38A)	121.7(8)	B(2)-C(1B)-H(1B2)	108.2
C(34A)-C(39A)-H(39A)	119.2	P(4)-C(1B)-H(1B2)	108.2
C(38A)-C(39A)-H(39A)	119.2	H(1B1)-C(1B)-H(1B2)	107.3
C(41A)-C(40A)-C(45A)	114.3(6)	B(2)-C(2B)-P(6)	114.7(4)
C(41A)-C(40A)-B(1)	121.5(6)	B(2)-C(2B)-H(2B1)	108.6
C(45A)-C(40A)-B(1)	124.1(6)	P(6)-C(2B)-H(2B1)	108.6

B(2)-C(2B)-H(2B2)	108.6	C(20B)-C(19B)-C(18B)	117.3(8)
P(6)-C(2B)-H(2B2)	108.6	C(20B)-C(19B)-H(19B)	121.4
H(2B1)-C(2B)-H(2B2)	107.6	C(18B)-C(19B)-H(19B)	121.3
B(2)-C(3B)-P(5)	114.3(4)	C(19B)-C(20B)-C(21B)	121.7(8)
B(2)-C(3B)-H(3B1)	108.7	C(19B)-C(20B)-H(20B)	119.1
P(5)-C(3B)-H(3B1)	108.7	C(21B)-C(20B)-H(20B)	119.1
B(2)-C(3B)-H(3B2)	108.7	C(16B)-C(21B)-C(20B)	120.7(7)
P(5)-C(3B)-H(3B2)	108.7	C(16B)-C(21B)-H(21B)	119.6
H(3B1)-C(3B)-H(3B2)	107.6	C(20B)-C(21B)-H(21B)	119.6
C(5B)-C(4B)-C(9B)	116.7(7)	C(23B)-C(22B)-C(27B)	117.9(7)
C(5B)-C(4B)-P(4)	123.0(6)	C(23B)-C(22B)-P(5)	121.9(6)
C(9B)-C(4B)-P(4)	120.2(6)	C(27B)-C(22B)-P(5)	120.1(7)
C(4B)-C(5B)-C(6B)	121.9(8)	C(22B)-C(23B)-C(24B)	120.3(8)
C(4B)-C(5B)-H(5B)	119.1	C(22B)-C(23B)-H(23B)	119.8
C(6B)-C(5B)-H(5B)	119.1	C(24B)-C(23B)-H(23B)	119.8
C(5B)-C(6B)-C(7B)	119.6(8)	C(25B)-C(24B)-C(23B)	119.9(9)
C(5B)-C(6B)-H(6B)	120.2	C(25B)-C(24B)-H(24B)	120.1
C(7B)-C(6B)-H(6B)	120.2	C(23B)-C(24B)-H(24B)	120.1
C(8B)-C(7B)-C(6B)	120.0(8)	C(24B)-C(25B)-C(26B)	120.8(9)
C(8B)-C(7B)-H(7B)	120.0	C(24B)-C(25B)-H(25B)	119.6
C(6B)-C(7B)-H(7B)	120.0	C(26B)-C(25B)-H(25B)	119.6
C(9B)-C(8B)-C(7B)	119.9(8)	C(27B)-C(26B)-C(25B)	120.1(9)
C(9B)-C(8B)-H(8B)	120.0	C(27B)-C(26B)-H(26B)	119.9
C(7B)-C(8B)-H(8B)	120.0	C(25B)-C(26B)-H(26B)	119.9
C(8B)-C(9B)-C(4B)	121.9(8)	C(22B)-C(27B)-C(26B)	121.0(9)
C(8B)-C(9B)-H(9B)	119.1	C(22B)-C(27B)-H(27B)	119.5
C(4B)-C(9B)-H(9B)	119.1	C(26B)-C(27B)-H(27B)	119.5
C(15B)-C(10B)-C(11B)	117.0(6)	C(33B)-C(28B)-C(29B)	119.0(7)
C(15B)-C(10B)-P(4)	121.2(6)	C(33B)-C(28B)-P(6)	114.8(6)
C(11B)-C(10B)-P(4)	121.8(6)	C(29B)-C(28B)-P(6)	126.2(6)
C(12B)-C(11B)-C(10B)	120.6(7)	C(30B)-C(29B)-C(28B)	119.9(7)
C(12B)-C(11B)-H(11B)	119.7	C(30B)-C(29B)-H(29B)	120.0
C(10B)-C(11B)-H(11B)	119.7	C(28B)-C(29B)-H(29B)	120.0
C(11B)-C(12B)-C(13B)	121.8(8)	C(29B)-C(30B)-C(31B)	121.0(8)
C(11B)-C(12B)-H(12B)	119.1	C(29B)-C(30B)-H(30B)	119.5
C(13B)-C(12B)-H(12B)	119.1	C(31B)-C(30B)-H(30B)	119.5
C(12B)-C(13B)-C(14B)	118.9(7)	C(32B)-C(31B)-C(30B)	119.9(8)
C(12B)-C(13B)-H(13B)	120.6	C(32B)-C(31B)-H(31B)	120.1
C(14B)-C(13B)-H(13B)	120.6	C(30B)-C(31B)-H(31B)	120.1
C(15B)-C(14B)-C(13B)	119.3(7)	C(33B)-C(32B)-C(31B)	119.9(8)
C(15B)-C(14B)-H(14B)	120.4	C(33B)-C(32B)-H(32B)	120.0
C(13B)-C(14B)-H(14B)	120.3	C(31B)-C(32B)-H(32B)	120.0
C(10B)-C(15B)-C(14B)	122.4(7)	C(32B)-C(33B)-C(28B)	120.2(7)
C(10B)-C(15B)-H(15B)	118.8	C(32B)-C(33B)-H(33B)	119.9
C(14B)-C(15B)-H(15B)	118.8	C(28B)-C(33B)-H(33B)	119.9
C(21B)-C(16B)-C(17B)	117.4(7)	C(35B)-C(34B)-C(39B)	115.0(7)
C(21B)-C(16B)-P(5)	123.1(6)	C(35B)-C(34B)-P(6)	123.5(7)
C(17B)-C(16B)-P(5)	119.4(6)	C(39B)-C(34B)-P(6)	121.5(6)
C(18B)-C(17B)-C(16B)	121.0(8)	C(34B)-C(35B)-C(36B)	123.7(8)
C(18B)-C(17B)-H(17B)	119.5	C(34B)-C(35B)-H(35B)	118.2
C(16B)-C(17B)-H(17B)	119.5	C(36B)-C(35B)-H(35B)	118.2
C(17B)-C(18B)-C(19B)	121.8(8)	C(37B)-C(36B)-C(35B)	119.2(9)
C(17B)-C(18B)-H(18B)	119.1	C(37B)-C(36B)-H(36B)	120.4
C(19B)-C(18B)-H(18B)	119.1	C(35B)-C(36B)-H(36B)	120.4

C(36B)-C(37B)-C(38B)	118.4(9)
C(36B)-C(37B)-H(37B)	120.8
C(38B)-C(37B)-H(37B)	120.8
C(39B)-C(38B)-C(37B)	120.4(9)
C(39B)-C(38B)-H(38B)	119.8
C(37B)-C(38B)-H(38B)	119.8
C(38B)-C(39B)-C(34B)	123.2(8)
C(38B)-C(39B)-H(39B)	118.4
C(34B)-C(39B)-H(39B)	118.4
C(41B)-C(40B)-C(45B)	115.3(6)
C(41B)-C(40B)-B(2)	122.1(6)
C(45B)-C(40B)-B(2)	122.6(6)
C(42B)-C(41B)-C(40B)	124.2(7)
C(42B)-C(41B)-H(41B)	117.9
C(40B)-C(41B)-H(41B)	117.9
C(41B)-C(42B)-C(43B)	119.2(7)
C(41B)-C(42B)-H(42B)	120.4
C(43B)-C(42B)-H(42B)	120.4
C(42B)-C(43B)-C(44B)	118.6(7)
C(42B)-C(43B)-H(43B)	120.7
C(44B)-C(43B)-H(43B)	120.7
C(45B)-C(44B)-C(43B)	120.6(7)
C(45B)-C(44B)-H(44B)	119.7
C(43B)-C(44B)-H(44B)	119.7
C(44B)-C(45B)-C(40B)	122.0(7)
C(44B)-C(45B)-H(45B)	119.0
C(40B)-C(45B)-H(45B)	119.0
C(102)-C(101)-C(106)	120.0
C(102)-C(101)-H(101)	120.3
C(106)-C(101)-H(101)	119.7
C(103)-C(102)-C(101)	120.0
C(103)-C(102)-H(102)	120.0
C(101)-C(102)-H(102)	120.0
C(104)-C(103)-C(102)	120.0
C(104)-C(103)-H(103)	120.0
C(102)-C(103)-H(103)	120.0
C(103)-C(104)-C(105)	120.0
C(103)-C(104)-H(104)	120.0
C(105)-C(104)-H(104)	120.0
C(106)-C(105)-C(104)	120.0
C(106)-C(105)-H(105)	120.0
C(104)-C(105)-H(105)	120.0
C(105)-C(106)-C(101)	120.0
C(105)-C(106)-H(106)	120.0
C(101)-C(106)-H(106)	120.0

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for BAQ07 (CCDC 160107). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

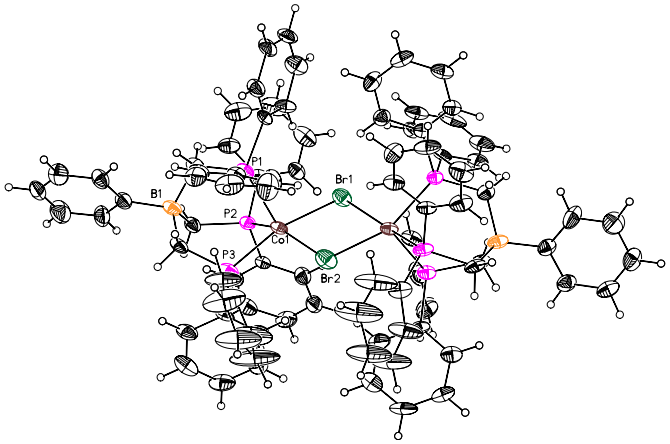
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	332(6)	308(6)	278(6)	-21(5)	-19(5)	17(5)
I(1)	547(4)	546(4)	308(3)	36(3)	-4(3)	118(3)
P(1)	355(13)	362(12)	322(12)	-20(10)	-36(10)	38(10)
P(2)	355(12)	272(12)	308(12)	21(9)	-10(10)	25(9)
P(3)	411(13)	333(12)	292(12)	3(10)	-28(10)	68(10)
B(1)	340(50)	320(50)	280(50)	10(40)	-10(40)	30(40)
C(1A)	290(40)	380(50)	310(40)	-110(40)	-20(40)	-50(40)
C(2A)	290(40)	270(40)	280(40)	-40(30)	30(30)	40(30)
C(3A)	370(50)	220(40)	400(50)	20(40)	-100(40)	0(40)
C(4A)	360(50)	290(50)	320(50)	0(40)	-20(40)	20(40)
C(5A)	590(60)	360(50)	460(50)	60(40)	120(40)	100(40)
C(6A)	740(60)	380(60)	560(60)	20(50)	0(50)	120(50)
C(7A)	590(60)	350(50)	640(60)	80(50)	-150(50)	-10(50)
C(8A)	600(60)	460(60)	350(50)	10(50)	-30(40)	-30(50)
C(9A)	530(50)	380(50)	350(50)	-30(40)	-40(40)	90(40)
C(10A)	340(50)	250(40)	340(50)	10(40)	-110(40)	50(40)
C(11A)	330(50)	750(60)	520(60)	-180(50)	-30(40)	50(50)
C(12A)	400(60)	1190(80)	590(70)	-190(60)	60(50)	130(60)
C(13A)	350(50)	750(70)	800(70)	40(60)	-60(50)	110(50)
C(14A)	380(60)	600(60)	660(60)	-190(50)	-90(50)	-60(50)
C(15A)	410(60)	630(60)	430(50)	-30(40)	-30(50)	40(50)
C(16A)	380(50)	260(50)	310(50)	-10(40)	0(40)	100(40)
C(17A)	390(50)	630(60)	410(50)	20(50)	30(40)	-90(40)
C(18A)	590(60)	800(70)	400(50)	-40(50)	-30(50)	70(60)
C(19A)	590(70)	470(60)	650(70)	-140(50)	-300(60)	70(50)
C(20A)	570(60)	520(60)	730(70)	180(50)	-120(50)	-90(50)
C(21A)	530(60)	420(50)	460(50)	60(40)	-240(50)	-50(40)
C(22A)	210(40)	310(40)	280(40)	0(40)	-80(40)	-20(30)
C(23A)	320(50)	410(50)	430(50)	40(40)	90(40)	80(40)
C(24A)	530(60)	320(50)	570(60)	170(40)	150(50)	60(40)
C(25A)	610(60)	260(50)	630(60)	60(50)	80(50)	90(40)
C(26A)	550(60)	510(60)	460(60)	-30(50)	160(50)	200(50)
C(27A)	510(50)	330(50)	350(50)	50(40)	90(40)	60(40)
C(28A)	430(50)	270(40)	240(50)	-30(40)	-20(40)	10(40)
C(29A)	680(60)	340(50)	290(50)	10(40)	-70(50)	10(50)
C(30A)	660(60)	450(60)	420(60)	-40(50)	-240(50)	0(50)
C(31A)	470(60)	430(60)	690(70)	-110(50)	-140(50)	0(40)
C(32A)	540(60)	360(50)	410(50)	60(40)	-140(50)	110(40)
C(33A)	390(50)	340(50)	350(50)	-50(40)	-110(40)	90(40)
C(34A)	480(50)	260(40)	250(50)	-20(40)	10(40)	60(40)
C(35A)	640(60)	520(60)	390(50)	-100(50)	-10(50)	170(50)
C(36A)	620(70)	790(70)	660(70)	-100(60)	-10(60)	360(50)
C(37A)	640(70)	680(70)	810(80)	-130(60)	40(60)	320(50)
C(38A)	950(80)	1000(80)	590(70)	-220(60)	150(60)	440(70)
C(39A)	710(70)	760(70)	410(60)	-30(50)	40(50)	340(50)
C(40A)	200(40)	460(50)	290(40)	-120(40)	-60(30)	60(40)
C(41A)	580(60)	270(50)	280(50)	40(40)	-90(40)	-40(40)

C(42A)	570(60)	330(50)	410(50)	50(40)	-50(50)	90(40)
C(43A)	550(60)	580(60)	180(40)	20(40)	-10(40)	230(50)
C(44A)	490(50)	390(50)	400(60)	-150(40)	-60(40)	30(40)
C(45A)	290(50)	390(50)	350(50)	30(40)	20(40)	-30(40)
Co(2)	285(6)	384(6)	410(6)	-17(5)	-51(5)	15(5)
I(2)	334(3)	646(4)	835(4)	-3(4)	-162(3)	-20(3)
P(4)	295(12)	403(13)	471(14)	19(11)	-26(11)	-4(10)
P(5)	367(12)	451(13)	374(12)	-42(11)	-54(10)	40(11)
P(6)	319(12)	367(13)	473(13)	-39(11)	-20(10)	11(10)
B(2)	230(50)	290(50)	390(50)	10(40)	-30(40)	20(40)
C(1B)	310(50)	490(50)	410(50)	-60(40)	-40(40)	0(40)
C(2B)	400(50)	330(40)	430(50)	10(40)	-40(40)	-60(40)
C(3B)	290(40)	360(50)	410(50)	-80(40)	50(40)	0(30)
C(4B)	310(50)	350(50)	470(50)	30(40)	10(40)	-30(40)
C(5B)	420(60)	540(60)	670(70)	-10(50)	20(50)	-70(40)
C(6B)	520(60)	720(70)	580(60)	-180(50)	20(50)	-100(50)
C(7B)	800(80)	880(70)	410(60)	-100(50)	80(60)	-50(60)
C(8B)	490(60)	870(70)	640(70)	-50(60)	170(60)	20(50)
C(9B)	390(60)	730(60)	450(60)	-40(50)	-30(50)	-80(50)
C(10B)	340(50)	320(50)	430(50)	-20(40)	-20(40)	-40(40)
C(11B)	330(50)	430(60)	800(70)	-140(50)	-50(50)	20(40)
C(12B)	430(60)	550(60)	760(60)	-60(60)	-110(50)	-190(50)
C(13B)	580(60)	440(60)	680(60)	-40(50)	-140(50)	-80(50)
C(14B)	460(60)	450(60)	990(80)	-120(50)	-120(50)	60(50)
C(15B)	340(50)	430(50)	590(60)	-70(50)	-110(40)	-50(40)
C(16B)	360(50)	460(50)	280(50)	-30(40)	-70(40)	170(40)
C(17B)	480(60)	490(60)	570(60)	-90(50)	10(50)	-20(50)
C(18B)	640(70)	460(60)	790(70)	-150(50)	100(60)	-70(50)
C(19B)	830(70)	410(60)	470(60)	-80(50)	20(50)	130(60)
C(20B)	580(60)	600(60)	420(50)	-40(50)	-60(50)	200(50)
C(21B)	490(60)	520(60)	350(50)	-90(40)	-140(40)	40(50)
C(22B)	330(50)	560(60)	410(50)	-50(40)	10(40)	180(40)
C(23B)	390(50)	710(60)	390(50)	20(50)	20(40)	90(50)
C(24B)	810(80)	820(70)	480(60)	170(60)	120(60)	190(60)
C(25B)	850(90)	950(90)	440(70)	40(60)	-210(60)	320(70)
C(26B)	650(70)	950(90)	700(80)	-210(70)	-220(60)	100(60)
C(27B)	600(60)	710(60)	420(60)	-60(50)	-190(50)	230(50)
C(28B)	300(50)	380(50)	490(50)	-40(40)	-60(40)	80(40)
C(29B)	460(60)	460(50)	420(50)	-20(40)	-70(40)	-30(40)
C(30B)	590(60)	550(60)	710(70)	150(50)	-130(60)	-40(50)
C(31B)	880(80)	400(60)	600(60)	140(50)	-90(60)	-40(60)
C(32B)	600(70)	500(60)	520(60)	30(50)	-120(50)	100(50)
C(33B)	410(50)	430(50)	580(60)	10(50)	10(50)	60(40)
C(34B)	320(50)	320(50)	540(60)	-40(40)	-10(40)	50(40)
C(35B)	440(60)	680(70)	1210(90)	-370(60)	310(60)	-20(50)
C(36B)	570(70)	890(80)	1380(100)	-460(70)	370(70)	-140(60)
C(37B)	820(80)	580(70)	680(70)	-110(60)	100(60)	210(60)
C(38B)	750(80)	670(70)	840(80)	-350(60)	-40(70)	-30(60)
C(39B)	460(60)	710(70)	730(70)	-260(60)	100(50)	40(50)
C(40B)	300(40)	340(50)	250(40)	10(40)	20(30)	40(40)
C(41B)	360(50)	260(50)	570(50)	40(40)	-70(40)	10(40)
C(42B)	350(50)	420(50)	530(50)	40(40)	-50(40)	-140(40)
C(43B)	310(50)	530(60)	450(50)	-130(50)	10(40)	-60(50)
C(44B)	410(50)	410(50)	350(50)	40(40)	100(40)	110(40)

C(45B)	230(50)	550(60)	430(50)	-20(40)	-70(40)	-50(40)

2: {[PhBP$_3$]Co(μ-Br)}$_2$

Contents



MJA09

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 163774. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 163774."

Table 1. Crystal data and structure refinement for MJA09 (CCDC 163774).

Empirical formula	$C_{90}H_{82}B_2Br_2Co_2P_6$
Formula weight	1648.68
Crystallization Solvent	Benzene/petroleum ether
Crystal Habit	Needle
Crystal size	0.22 x 0.11 x 0.05 mm^3
Crystal color	Red

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 3832 reflections used in lattice determination	2.39 to 27.78°
Unit cell dimensions	a = 22.214(3) Å b = 19.286(3) Å c = 18.008(3) Å
Volume	7715.0(19) $Å^3$
Z	4
Crystal system	Orthorhombic
Space group	Pbcn
Density (calculated)	1.419 Mg/m^3
F(000)	3384
Data collection program	Bruker SMART
θ range for data collection	1.83 to 28.73°
Completeness to θ = 28.73°	92.6 %
Index ranges	$0 \le h \le 29$, $0 \le k \le 26$, $0 \le l \le 24$
Data collection scan type	ω scans at 4 ϕ settings
Data reduction program	Bruker SAINT v6.2
Reflections collected	9263
Independent reflections	9263 [R_{int}= 0.0000]
Absorption coefficient	1.637 mm^{-1}
Absorption correction	None
Max. and min. transmission (calculated)	0.9153 and 0.7126

Table 1 (cont.)

Structure solution and Refinement

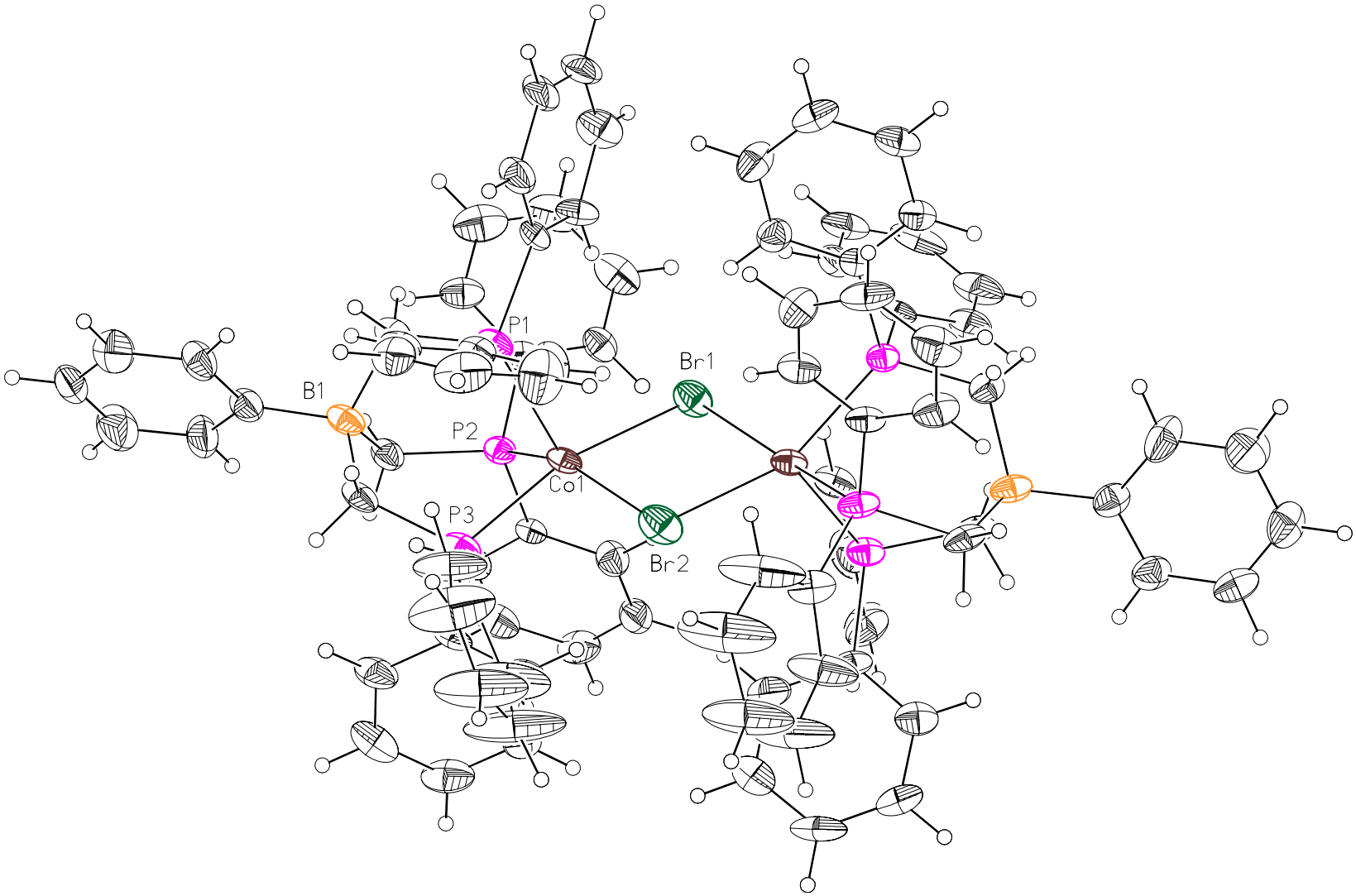
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	9263 / 0 / 461
Treatment of hydrogen atoms	Restrained
Goodness-of-fit on F^2	1.534
Final R indices [$I>2\sigma(I)$, 4429 reflections]	R1 = 0.0695, *w*R2 = 0.0965
R indices (all data)	R1 = 0.1432, *w*R2 = 0.1012
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.000
Average shift/error	0.000
Largest diff. peak and hole	2.231 and -1.641 e.Å^{-3}

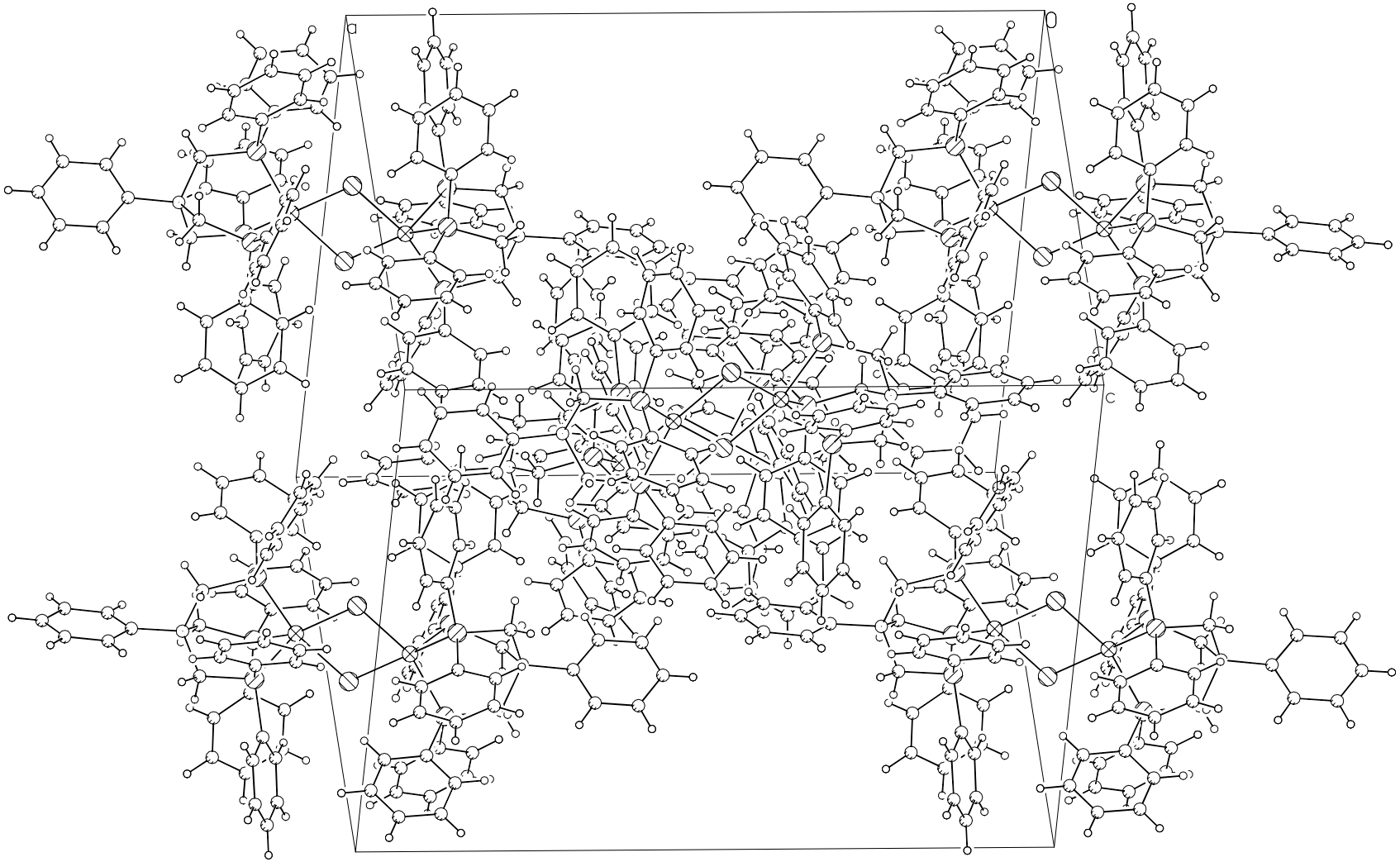
Special Refinement Details

All peaks in the final difference Fourier greater than 1e$^-$/Å^3 lie within 1Å of either cobalt or bromine positions.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


P1
B1
Br1
P2
Co1
P3
Br2



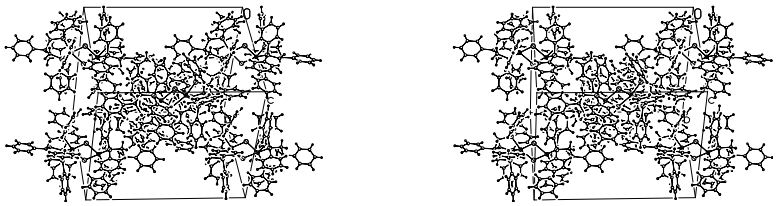


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MJA09 (CCDC 163774). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Co(1)	793(1)	2478(1)	2217(1)	23(1)
Br(1)	0	1665(1)	2500	36(1)
Br(2)	0	3299(1)	2500	42(1)
P(1)	1457(1)	2301(1)	3205(1)	27(1)
P(2)	1280(1)	1734(1)	1468(1)	23(1)
P(3)	1367(1)	3316(1)	1735(1)	28(1)
B(1)	2390(3)	2387(4)	2021(3)	30(2)
C(1)	2194(2)	2089(3)	2857(3)	29(1)
C(2)	2060(2)	1956(3)	1334(3)	29(1)
C(3)	2156(2)	3208(3)	1947(3)	31(2)
C(4)	3111(2)	2364(3)	1910(3)	32(2)
C(5)	3504(2)	2549(3)	2468(3)	37(1)
C(6)	4118(2)	2569(3)	2369(3)	45(2)
C(7)	4375(2)	2389(4)	1713(3)	45(2)
C(8)	3992(3)	2191(4)	1150(3)	56(2)
C(9)	3381(3)	2173(3)	1256(3)	49(2)
C(10)	1548(3)	3075(3)	3794(3)	28(1)
C(11)	2087(3)	3400(3)	3956(3)	35(2)
C(12)	2101(3)	3994(3)	4379(3)	43(2)
C(13)	1584(4)	4286(3)	4646(3)	51(2)
C(14)	1039(3)	3968(4)	4503(4)	58(2)
C(15)	1011(3)	3369(4)	4065(3)	51(2)
C(16)	1349(2)	1616(3)	3913(3)	28(1)
C(17)	1560(2)	1702(3)	4632(3)	40(2)
C(18)	1529(3)	1151(4)	5126(3)	48(2)
C(19)	1295(3)	534(3)	4926(3)	43(2)
C(20)	1083(3)	454(3)	4216(4)	44(2)
C(21)	1102(2)	995(3)	3707(3)	32(2)
C(22)	1291(3)	819(3)	1753(3)	26(1)
C(23)	1809(3)	496(3)	2013(3)	35(2)
C(24)	1800(3)	-187(3)	2220(3)	48(2)
C(25)	1295(3)	-575(3)	2174(3)	48(2)
C(26)	767(3)	-266(3)	1924(3)	41(2)
C(27)	767(3)	419(3)	1714(3)	29(2)
C(28)	946(2)	1639(3)	536(3)	21(1)
C(29)	1309(3)	1540(3)	-73(3)	30(1)
C(30)	1059(3)	1436(3)	-769(3)	37(2)
C(31)	445(3)	1444(3)	-852(3)	39(2)
C(32)	90(3)	1538(3)	-257(3)	38(2)
C(33)	335(2)	1642(3)	436(3)	32(2)
C(34)	1291(3)	3354(3)	709(3)	25(1)
C(35)	1778(3)	3519(3)	262(3)	40(2)
C(36)	1688(3)	3549(3)	-501(4)	50(2)
C(37)	1126(3)	3446(3)	-800(4)	46(2)
C(38)	656(3)	3308(3)	-355(3)	38(2)
C(39)	746(3)	3251(3)	389(3)	33(2)
C(40)	1180(3)	4208(3)	1970(3)	36(2)

C(41)	1387(3)	4512(3)	2604(3)	65(2)
C(42)	1292(4)	5198(4)	2764(4)	97(3)
C(43)	960(4)	5610(4)	2314(4)	103(4)
C(44)	678(5)	5306(4)	1685(4)	117(4)
C(45)	818(4)	4616(4)	1536(4)	91(3)

Table 3. Selected bond lengths [Å] and angles [°] for MJA09 (CCDC 163774).

Co(1)-P(3)	2.2345(17)	Br(1)-Co(1)-Br(2)	81.33(3)
Co(1)-P(2)	2.2467(16)	Co(1)-Br(1)-Co(1)#1	98.97(5)
Co(1)-P(1)	2.3361(16)	Co(1)-Br(2)-Co(1)#1	98.37(5)
Co(1)-Br(1)	2.4127(9)		
Co(1)-Br(2)	2.4235(10)		
Br(1)-Co(1)#1	2.4127(9)		
Br(2)-Co(1)#1	2.4235(10)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 4. Bond lengths [Å] and angles [°] for MJA09 (CCDC 163774).

Co(1)-P(3)	2.2345(17)	C(17)-H(17)	0.9500
Co(1)-P(2)	2.2467(16)	C(18)-C(19)	1.347(8)
Co(1)-P(1)	2.3361(16)	C(18)-H(18)	0.9500
Co(1)-Br(1)	2.4127(9)	C(19)-C(20)	1.372(7)
Co(1)-Br(2)	2.4235(10)	C(19)-H(19)	0.9500
Br(1)-Co(1)#1	2.4127(9)	C(20)-C(21)	1.388(7)
Br(2)-Co(1)#1	2.4235(10)	C(20)-H(20)	0.9500
P(1)-C(1)	1.800(5)	C(21)-H(21)	0.9500
P(1)-C(10)	1.843(5)	C(22)-C(23)	1.390(7)
P(1)-C(16)	1.852(5)	C(22)-C(27)	1.399(7)
P(2)-C(2)	1.800(5)	C(23)-C(24)	1.370(8)
P(2)-C(22)	1.837(5)	C(23)-H(23)	0.9500
P(2)-C(28)	1.843(5)	C(24)-C(25)	1.350(8)
P(3)-C(3)	1.806(5)	C(24)-H(24)	0.9500
P(3)-C(40)	1.819(6)	C(25)-C(26)	1.389(8)
P(3)-C(34)	1.856(5)	C(25)-H(25)	0.9500
B(1)-C(4)	1.614(7)	C(26)-C(27)	1.375(7)
B(1)-C(2)	1.662(7)	C(26)-H(26)	0.9500
B(1)-C(3)	1.671(8)	C(27)-H(27)	0.9500
B(1)-C(1)	1.669(7)	C(28)-C(33)	1.369(6)
C(1)-H(1A)	0.9900	C(28)-C(29)	1.377(7)
C(1)-H(1B)	0.9900	C(29)-C(30)	1.385(7)
C(2)-H(2A)	0.9900	C(29)-H(29)	0.9500
C(2)-H(2B)	0.9900	C(30)-C(31)	1.372(7)
C(3)-H(3A)	0.9900	C(30)-H(30)	0.9500
C(3)-H(3B)	0.9900	C(31)-C(32)	1.343(7)
C(4)-C(5)	1.377(6)	C(31)-H(31)	0.9500
C(4)-C(9)	1.373(7)	C(32)-C(33)	1.375(7)
C(5)-C(6)	1.376(6)	C(32)-H(32)	0.9500
C(5)-H(5)	0.9500	C(33)-H(33)	0.9500
C(6)-C(7)	1.357(7)	C(34)-C(39)	1.357(7)
C(6)-H(6)	0.9500	C(34)-C(35)	1.386(7)
C(7)-C(8)	1.379(7)	C(35)-C(36)	1.389(7)
C(7)-H(7)	0.9500	C(35)-H(35)	0.9500
C(8)-C(9)	1.370(7)	C(36)-C(37)	1.374(8)
C(8)-H(8)	0.9500	C(36)-H(36)	0.9500
C(9)-H(9)	0.9500	C(37)-C(38)	1.344(8)
C(10)-C(11)	1.383(7)	C(37)-H(37)	0.9500
C(10)-C(15)	1.408(7)	C(38)-C(39)	1.359(7)
C(11)-C(12)	1.376(7)	C(38)-H(38)	0.9500
C(11)-H(11)	0.9500	C(39)-H(39)	0.9500
C(12)-C(13)	1.368(8)	C(40)-C(45)	1.370(9)
C(12)-H(12)	0.9500	C(40)-C(41)	1.363(7)
C(13)-C(14)	1.381(8)	C(41)-C(42)	1.371(8)
C(13)-H(13)	0.9500	C(41)-H(41)	0.9500
C(14)-C(15)	1.400(8)	C(42)-C(43)	1.353(9)
C(14)-H(14)	0.9500	C(42)-H(42)	0.9500
C(15)-H(15)	0.9500	C(43)-C(44)	1.421(10)
C(16)-C(21)	1.368(7)	C(43)-H(43)	0.9500
C(16)-C(17)	1.386(7)	C(44)-C(45)	1.394(9)
C(17)-C(18)	1.388(8)	C(44)-H(44)	0.9500

C(45)-H(45)	0.9500	P(3)-C(3)-H(3B)	108.4
		H(3A)-C(3)-H(3B)	107.5
P(3)-Co(1)-P(2)	87.42(6)	C(5)-C(4)-C(9)	114.8(5)
P(3)-Co(1)-P(1)	92.35(6)	C(5)-C(4)-B(1)	122.1(5)
P(2)-Co(1)-P(1)	93.44(6)	C(9)-C(4)-B(1)	123.2(5)
P(3)-Co(1)-Br(1)	165.70(5)	C(4)-C(5)-C(6)	122.7(5)
P(2)-Co(1)-Br(1)	93.63(5)	C(4)-C(5)-H(5)	118.7
P(1)-Co(1)-Br(1)	101.81(4)	C(6)-C(5)-H(5)	118.7
P(3)-Co(1)-Br(2)	91.35(5)	C(5)-C(6)-C(7)	121.6(5)
P(2)-Co(1)-Br(2)	153.37(5)	C(5)-C(6)-H(6)	119.2
P(1)-Co(1)-Br(2)	113.19(4)	C(7)-C(6)-H(6)	119.2
Br(1)-Co(1)-Br(2)	81.33(3)	C(8)-C(7)-C(6)	116.8(6)
Co(1)-Br(1)-Co(1)#1	98.97(5)	C(8)-C(7)-H(7)	121.6
Co(1)-Br(2)-Co(1)#1	98.37(5)	C(6)-C(7)-H(7)	121.6
C(1)-P(1)-C(10)	106.5(2)	C(9)-C(8)-C(7)	121.1(6)
C(1)-P(1)-C(16)	101.3(2)	C(9)-C(8)-H(8)	119.5
C(10)-P(1)-C(16)	101.2(2)	C(7)-C(8)-H(8)	119.5
C(1)-P(1)-Co(1)	110.02(17)	C(4)-C(9)-C(8)	123.0(6)
C(10)-P(1)-Co(1)	112.94(18)	C(4)-C(9)-H(9)	118.5
C(16)-P(1)-Co(1)	123.19(19)	C(8)-C(9)-H(9)	118.5
C(2)-P(2)-C(22)	104.6(3)	C(11)-C(10)-C(15)	118.5(5)
C(2)-P(2)-C(28)	106.8(2)	C(11)-C(10)-P(1)	125.7(5)
C(22)-P(2)-C(28)	99.5(2)	C(15)-C(10)-P(1)	115.7(4)
C(2)-P(2)-Co(1)	113.01(18)	C(12)-C(11)-C(10)	121.0(6)
C(22)-P(2)-Co(1)	116.90(18)	C(12)-C(11)-H(11)	119.5
C(28)-P(2)-Co(1)	114.53(18)	C(10)-C(11)-H(11)	119.5
C(3)-P(3)-C(40)	106.4(3)	C(11)-C(12)-C(13)	121.2(6)
C(3)-P(3)-C(34)	107.6(3)	C(11)-C(12)-H(12)	119.4
C(40)-P(3)-C(34)	100.1(3)	C(13)-C(12)-H(12)	119.4
C(3)-P(3)-Co(1)	112.85(18)	C(12)-C(13)-C(14)	119.2(6)
C(40)-P(3)-Co(1)	117.6(2)	C(12)-C(13)-H(13)	120.4
C(34)-P(3)-Co(1)	111.23(18)	C(14)-C(13)-H(13)	120.4
C(4)-B(1)-C(2)	109.4(5)	C(13)-C(14)-C(15)	120.7(6)
C(4)-B(1)-C(3)	108.9(5)	C(13)-C(14)-H(14)	119.6
C(2)-B(1)-C(3)	106.1(4)	C(15)-C(14)-H(14)	119.6
C(4)-B(1)-C(1)	111.2(4)	C(10)-C(15)-C(14)	119.4(6)
C(2)-B(1)-C(1)	112.5(4)	C(10)-C(15)-H(15)	120.3
C(3)-B(1)-C(1)	108.5(5)	C(14)-C(15)-H(15)	120.3
B(1)-C(1)-P(1)	118.2(4)	C(21)-C(16)-C(17)	119.5(5)
B(1)-C(1)-H(1A)	107.7	C(21)-C(16)-P(1)	119.3(4)
P(1)-C(1)-H(1A)	107.7	C(17)-C(16)-P(1)	121.0(5)
B(1)-C(1)-H(1B)	107.7	C(16)-C(17)-C(18)	119.4(6)
P(1)-C(1)-H(1B)	107.7	C(16)-C(17)-H(17)	120.3
H(1A)-C(1)-H(1B)	107.1	C(18)-C(17)-H(17)	120.3
B(1)-C(2)-P(2)	116.4(4)	C(19)-C(18)-C(17)	121.5(6)
B(1)-C(2)-H(2A)	108.2	C(19)-C(18)-H(18)	119.2
P(2)-C(2)-H(2A)	108.2	C(17)-C(18)-H(18)	119.2
B(1)-C(2)-H(2B)	108.2	C(18)-C(19)-C(20)	118.7(6)
P(2)-C(2)-H(2B)	108.2	C(18)-C(19)-H(19)	120.6
H(2A)-C(2)-H(2B)	107.3	C(20)-C(19)-H(19)	120.6
B(1)-C(3)-P(3)	115.4(4)	C(21)-C(20)-C(19)	121.4(6)
B(1)-C(3)-H(3A)	108.4	C(21)-C(20)-H(20)	119.3
P(3)-C(3)-H(3A)	108.4	C(19)-C(20)-H(20)	119.3
B(1)-C(3)-H(3B)	108.4	C(16)-C(21)-C(20)	119.4(5)

C(16)-C(21)-H(21)	120.3	C(34)-C(39)-H(39)	118.7
C(20)-C(21)-H(21)	120.3	C(38)-C(39)-H(39)	118.7
C(23)-C(22)-C(27)	117.3(5)	C(45)-C(40)-C(41)	115.4(6)
C(23)-C(22)-P(2)	122.4(5)	C(45)-C(40)-P(3)	123.0(5)
C(27)-C(22)-P(2)	120.3(4)	C(41)-C(40)-P(3)	121.6(5)
C(22)-C(23)-C(24)	120.7(6)	C(42)-C(41)-C(40)	122.6(6)
C(22)-C(23)-H(23)	119.7	C(42)-C(41)-H(41)	118.7
C(24)-C(23)-H(23)	119.7	C(40)-C(41)-H(41)	118.7
C(25)-C(24)-C(23)	121.9(6)	C(43)-C(42)-C(41)	121.6(7)
C(25)-C(24)-H(24)	119.0	C(43)-C(42)-H(42)	119.2
C(23)-C(24)-H(24)	119.0	C(41)-C(42)-H(42)	119.2
C(24)-C(25)-C(26)	118.9(6)	C(44)-C(43)-C(42)	118.4(7)
C(24)-C(25)-H(25)	120.5	C(44)-C(43)-H(43)	120.8
C(26)-C(25)-H(25)	120.5	C(42)-C(43)-H(43)	120.8
C(27)-C(26)-C(25)	120.1(6)	C(43)-C(44)-C(45)	116.7(8)
C(27)-C(26)-H(26)	119.9	C(43)-C(44)-H(44)	121.7
C(25)-C(26)-H(26)	119.9	C(45)-C(44)-H(44)	121.7
C(26)-C(27)-C(22)	121.0(6)	C(40)-C(45)-C(44)	124.7(7)
C(26)-C(27)-H(27)	119.5	C(40)-C(45)-H(45)	117.6
C(22)-C(27)-H(27)	119.5	C(44)-C(45)-H(45)	117.6
C(33)-C(28)-C(29)	118.5(5)		
C(33)-C(28)-P(2)	121.3(4)		
C(29)-C(28)-P(2)	120.2(4)		
C(30)-C(29)-C(28)	120.4(6)		
C(30)-C(29)-H(29)	119.8		
C(28)-C(29)-H(29)	119.8		
C(29)-C(30)-C(31)	119.7(6)		
C(29)-C(30)-H(30)	120.2		
C(31)-C(30)-H(30)	120.2		
C(32)-C(31)-C(30)	119.9(6)		
C(32)-C(31)-H(31)	120.0		
C(30)-C(31)-H(31)	120.0		
C(31)-C(32)-C(33)	120.7(6)		
C(31)-C(32)-H(32)	119.6		
C(33)-C(32)-H(32)	119.6		
C(28)-C(33)-C(32)	120.8(6)		
C(28)-C(33)-H(33)	119.6		
C(32)-C(33)-H(33)	119.6		
C(39)-C(34)-C(35)	118.8(5)		
C(39)-C(34)-P(3)	120.0(4)		
C(35)-C(34)-P(3)	121.1(4)		
C(36)-C(35)-C(34)	118.3(6)		
C(36)-C(35)-H(35)	120.9		
C(34)-C(35)-H(35)	120.9		
C(35)-C(36)-C(37)	120.8(6)		
C(35)-C(36)-H(36)	119.6		
C(37)-C(36)-H(36)	119.6		
C(38)-C(37)-C(36)	120.1(6)		
C(38)-C(37)-H(37)	119.9		
C(36)-C(37)-H(37)	119.9		
C(37)-C(38)-C(39)	119.3(6)		
C(37)-C(38)-H(38)	120.4		
C(39)-C(38)-H(38)	120.4		
C(34)-C(39)-C(38)	122.7(6)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for MJA09 (CCDC 163774). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	347(4)	192(3)	143(3)	8(4)	8(3)	-37(4)
Br(1)	427(6)	269(5)	373(6)	0	78(5)	0
Br(2)	552(7)	228(5)	474(6)	0	94(5)	0
P(1)	375(10)	253(9)	167(8)	12(7)	18(7)	-63(7)
P(2)	280(9)	232(8)	176(8)	6(7)	-8(7)	-21(7)
P(3)	432(10)	250(8)	171(8)	10(8)	-35(7)	-108(8)
B(1)	420(40)	280(50)	180(40)	10(30)	-30(30)	-130(30)
C(1)	400(40)	280(30)	200(30)	-10(30)	-30(30)	-110(30)
C(2)	320(40)	350(40)	200(30)	20(30)	10(30)	-80(30)
C(3)	410(40)	400(40)	120(30)	30(30)	-40(30)	-190(30)
C(4)	330(30)	340(40)	280(30)	30(30)	-10(30)	-90(30)
C(5)	380(30)	370(30)	360(30)	-20(40)	20(30)	-140(40)
C(6)	480(40)	370(40)	490(40)	-50(40)	-100(30)	-160(40)
C(7)	350(40)	610(50)	380(40)	130(40)	60(30)	-120(40)
C(8)	520(50)	820(60)	340(40)	20(40)	70(40)	-110(40)
C(9)	300(40)	810(60)	370(40)	100(40)	-30(30)	-160(40)
C(10)	390(40)	310(40)	140(30)	-20(30)	-50(30)	-60(30)
C(11)	500(40)	370(40)	190(30)	40(30)	-10(30)	-50(30)
C(12)	510(50)	390(40)	380(40)	-40(30)	-170(40)	-110(40)
C(13)	860(60)	340(40)	340(40)	-150(30)	-190(40)	10(40)
C(14)	550(50)	680(50)	530(50)	-240(40)	90(40)	40(40)
C(15)	480(50)	630(50)	420(40)	-240(40)	0(30)	-140(40)
C(16)	280(40)	370(40)	190(30)	70(30)	80(30)	-20(30)
C(17)	400(40)	500(40)	300(40)	70(40)	-50(30)	-200(40)
C(18)	430(40)	810(60)	210(40)	170(40)	10(30)	-180(40)
C(19)	480(50)	480(40)	320(40)	200(40)	150(30)	80(40)
C(20)	600(50)	230(40)	470(50)	-20(30)	80(40)	30(30)
C(21)	510(40)	270(30)	170(30)	40(30)	10(30)	30(30)
C(22)	410(40)	240(30)	130(30)	-60(30)	10(30)	50(30)
C(23)	520(40)	310(40)	210(40)	-20(30)	-20(30)	60(30)
C(24)	750(60)	430(40)	250(40)	-90(40)	-70(40)	140(40)
C(25)	940(60)	250(40)	260(40)	-80(30)	90(40)	70(40)
C(26)	640(50)	340(40)	240(40)	-100(30)	100(40)	-110(40)
C(27)	350(40)	250(30)	280(40)	-20(30)	80(30)	-20(30)
C(28)	280(30)	180(30)	190(30)	30(30)	10(30)	-20(30)
C(29)	380(40)	270(30)	250(30)	-20(30)	30(30)	-50(30)
C(30)	580(50)	300(40)	230(40)	-40(30)	60(30)	-60(30)
C(31)	490(50)	330(40)	360(40)	30(30)	-190(40)	-100(30)
C(32)	320(40)	530(40)	300(40)	90(30)	-30(30)	-110(30)
C(33)	310(40)	330(40)	310(40)	-10(30)	10(30)	-60(30)
C(34)	430(40)	200(30)	130(30)	30(30)	0(30)	-80(30)
C(35)	550(50)	440(40)	200(40)	60(30)	-40(30)	-110(30)
C(36)	710(50)	410(40)	370(50)	30(40)	160(40)	-100(40)
C(37)	750(60)	350(40)	280(40)	-20(30)	-190(40)	-50(40)
C(38)	380(40)	390(40)	360(40)	100(40)	-70(30)	-10(30)
C(39)	510(40)	280(40)	200(30)	30(30)	-20(30)	-20(30)
C(40)	580(50)	240(40)	260(40)	90(30)	-50(30)	-110(30)

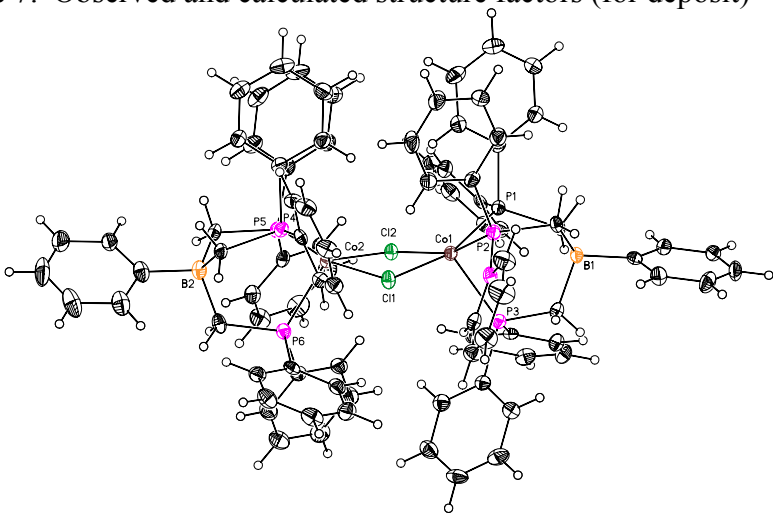
C(41)	1390(70)	310(40)	250(40)	-30(30)	-230(40)	200(40)
C(42)	1810(90)	480(50)	610(60)	-250(50)	-620(60)	250(60)
C(43)	2280(120)	220(40)	580(60)	-80(40)	-480(70)	160(60)
C(44)	2640(130)	270(50)	600(60)	-10(40)	-620(70)	370(60)
C(45)	2050(100)	300(40)	370(50)	-50(40)	-300(60)	30(60)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for MJA09 (CCDC 163774).

	x	y	z	U_{iso}
H(1A)	2493	2261	3220	35
H(1B)	2229	1578	2846	35
H(2A)	2288	1522	1249	34
H(2B)	2092	2238	877	34
H(3A)	2395	3439	1554	37
H(3B)	2243	3450	2420	37
H(5)	3344	2668	2941	44
H(6)	4367	2711	2769	54
H(7)	4799	2400	1646	53
H(8)	4154	2065	681	67
H(9)	3133	2022	858	59
H(11)	2452	3210	3773	42
H(12)	2477	4206	4486	51
H(13)	1599	4703	4927	62
H(14)	679	4157	4705	70
H(15)	633	3163	3952	61
H(17)	1724	2134	4785	48
H(18)	1676	1210	5618	58
H(19)	1276	162	5271	51
H(20)	921	20	4069	52
H(21)	945	935	3221	38
H(23)	2174	752	2047	41
H(24)	2159	-395	2401	57
H(25)	1300	-1051	2310	58
H(26)	406	-529	1897	49
H(27)	405	624	1539	35
H(29)	1734	1543	-17	36
H(30)	1312	1360	-1187	45
H(31)	272	1384	-1330	47
H(32)	-335	1532	-315	46
H(33)	77	1717	849	38
H(35)	2163	3608	471	48
H(36)	2019	3643	-819	60
H(37)	1071	3472	-1323	55
H(38)	264	3251	-559	45
H(39)	414	3134	696	40
H(41)	1606	4237	2949	78
H(42)	1463	5389	3202	116
H(43)	918	6091	2416	123
H(44)	406	5561	1382	141
H(45)	651	4413	1101	109

3: {[PhBP$_3$]Co(μ-Cl)}$_2$

Contents



MJA08

Note: The crystallographic data has been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 163590. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 163590."

Table 1. Crystal data and structure refinement for MJA08 (CCDC 163590).

Empirical formula	$C_{90}H_{82}B_2Cl_2Co_2P_6 \cdot 2(C_6H_6)$
Formula weight	1715.97
Crystallization Solvent	Benzene/petroleum ether
Crystal Habit	Block
Crystal size	0.22 x 0.19 x 0.07 mm^3
Crystal color	Red/Brown

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 16594 reflections used in lattice determination	2.18 to 28.13°
Unit cell dimensions	a = 26.340(3) Å b = 13.2151(14) Å β= 117.909(2)° c = 28.015(3) Å
Volume	8617.6(16) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.323 Mg/m^3
F(000)	3576
Data collection program	Bruker SMART
θ range for data collection	1.46 to 28.63°
Completeness to θ = 28.63°	93.1 %
Index ranges	$-34 \le h \le 33$, $-16 \le k \le 17$, $-37 \le l \le 36$
Data collection scan type	ω scans at 4 ϕ settings
Data reduction program	Bruker SAINT v6.2
Reflections collected	106341
Independent reflections	20585 [R_{int}= 0.1020]
Absorption coefficient	0.607 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9564 and 0.8770

Table 1 (cont.)

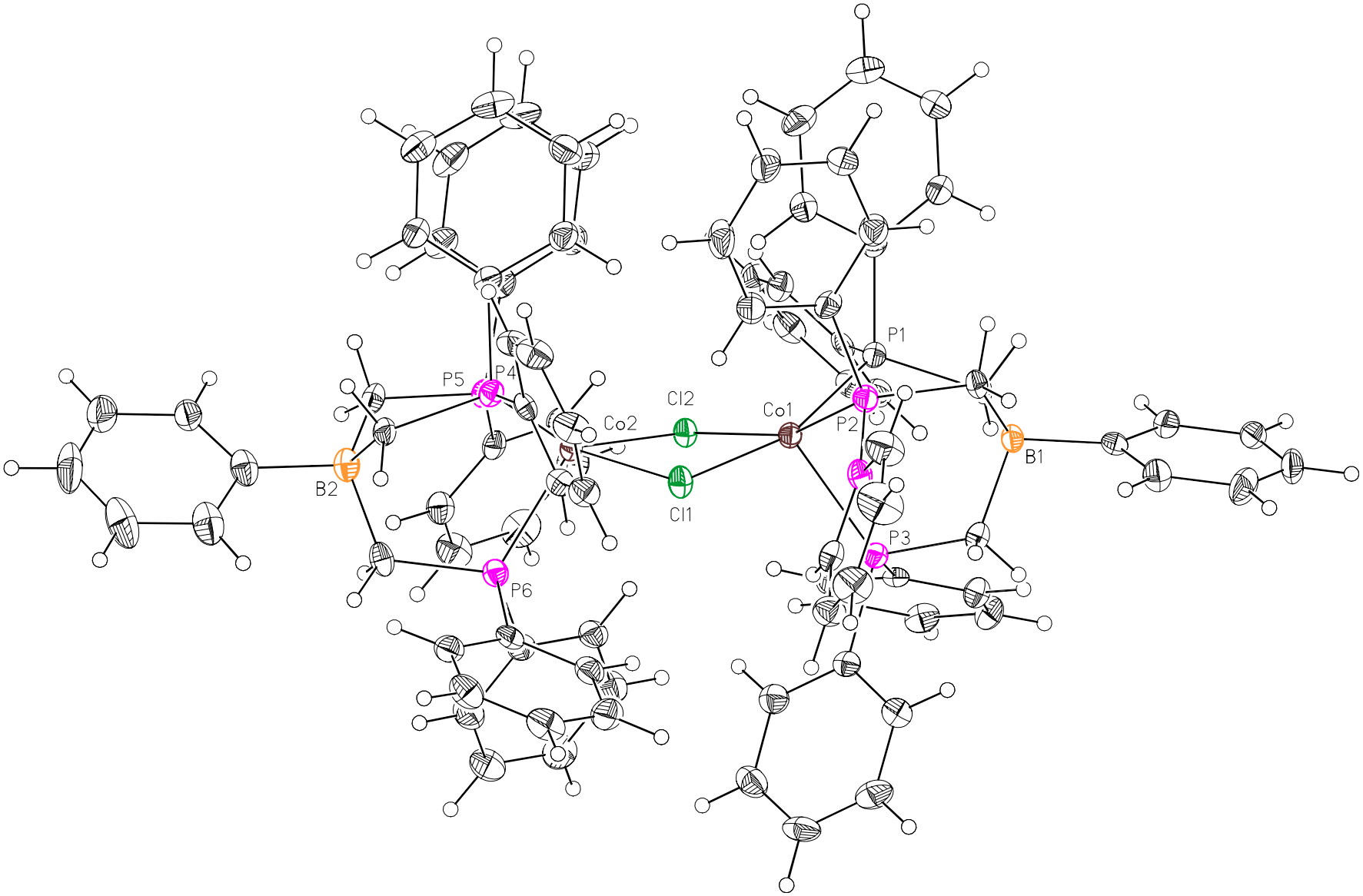
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	20585 / 0 / 1027
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.028
Final R indices [$I>2\sigma(I)$, 11762 reflections]	R1 = 0.0468, *w*R2 = 0.0660
R indices (all data)	R1 = 0.0995, *w*R2 = 0.0724
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	0.821 and -0.495 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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P4
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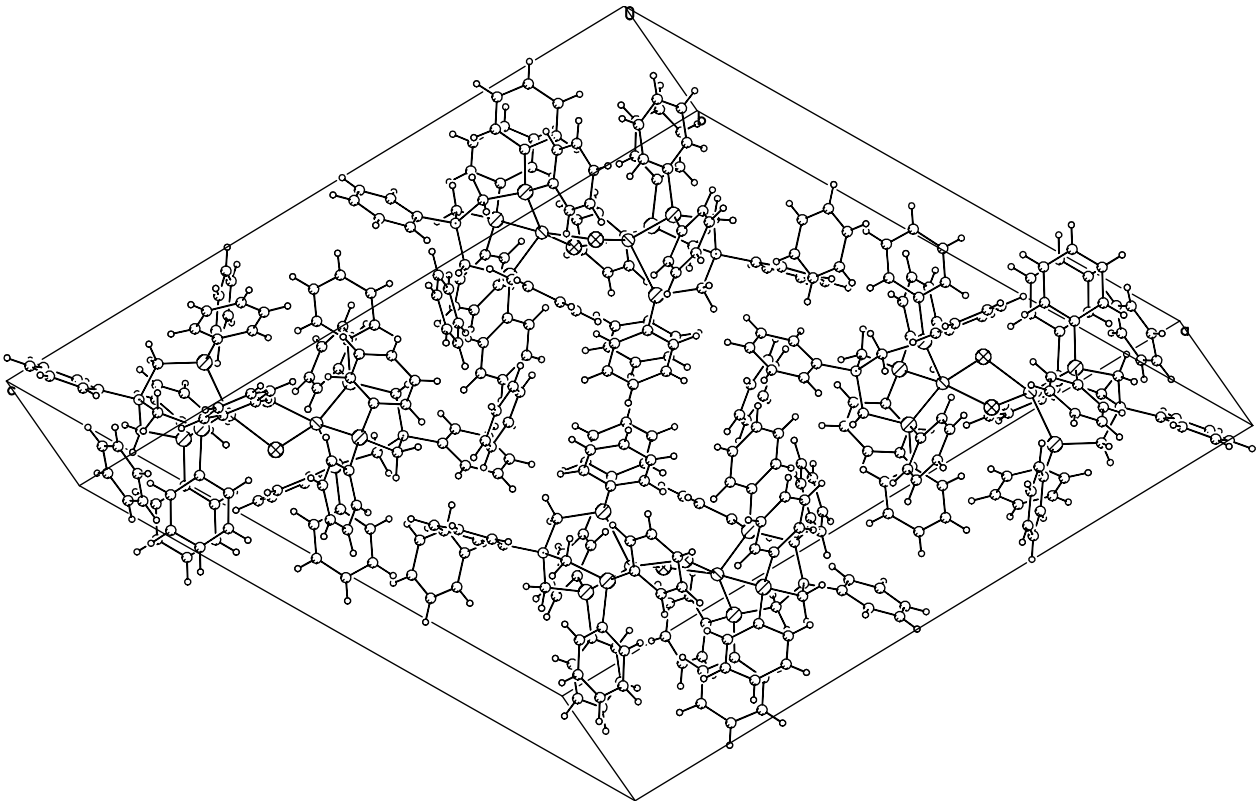
Co1
Co2
Cl1
Cl2
B1
B2



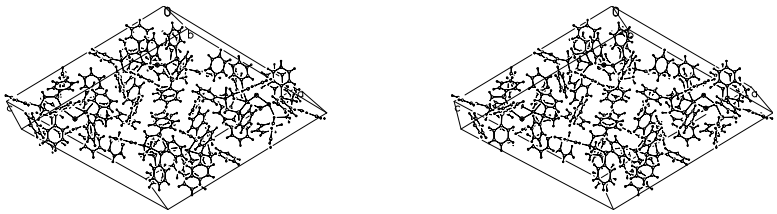


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MJA08 (CCDC 163590). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Co(1)	3011(1)	2701(1)	2961(1)	16(1)
Co(2)	2075(1)	2757(1)	3526(1)	16(1)
Cl(1)	2441(1)	3828(1)	3108(1)	20(1)
Cl(2)	2823(1)	1763(1)	3561(1)	18(1)
P(1)	3319(1)	1349(1)	2699(1)	17(1)
P(2)	2866(1)	3464(1)	2192(1)	18(1)
P(3)	3969(1)	3338(1)	3446(1)	16(1)
P(4)	1741(1)	1484(1)	3819(1)	18(1)
P(5)	1172(1)	3316(1)	3048(1)	18(1)
P(6)	2234(1)	3678(1)	4295(1)	18(1)
B(1)	4021(1)	2777(2)	2457(1)	17(1)
B(2)	1070(1)	3028(2)	4050(1)	21(1)
C(1)	3956(1)	1600(2)	2630(1)	18(1)
C(2)	3390(1)	3133(2)	1965(1)	20(1)
C(3)	4228(1)	3600(2)	2967(1)	17(1)
C(4)	1163(1)	1811(2)	3974(1)	20(1)
C(5)	831(1)	3626(2)	3461(1)	20(1)
C(6)	1677(1)	3523(2)	4504(1)	21(1)
C(7)	4510(1)	2810(2)	2255(1)	19(1)
C(8)	4615(1)	3702(2)	2040(1)	26(1)
C(9)	5053(1)	3788(2)	1899(1)	31(1)
C(10)	5414(1)	2975(2)	1967(1)	30(1)
C(11)	5327(1)	2081(2)	2178(1)	24(1)
C(12)	4885(1)	2008(2)	2316(1)	22(1)
C(13)	3471(1)	243(2)	3142(1)	17(1)
C(14)	4023(1)	8(2)	3542(1)	23(1)
C(15)	4122(1)	-827(2)	3874(1)	25(1)
C(16)	3670(1)	-1437(2)	3818(1)	25(1)
C(17)	3117(1)	-1221(2)	3422(1)	25(1)
C(18)	3020(1)	-393(2)	3091(1)	22(1)
C(19)	2789(1)	763(2)	2066(1)	20(1)
C(20)	2957(1)	113(2)	1773(1)	25(1)
C(21)	2557(1)	-406(2)	1327(1)	32(1)
C(22)	1981(1)	-309(2)	1175(1)	37(1)
C(23)	1801(1)	317(2)	1462(1)	33(1)
C(24)	2205(1)	853(2)	1907(1)	25(1)
C(25)	2150(1)	3276(2)	1618(1)	20(1)
C(26)	2051(1)	2739(2)	1153(1)	26(1)
C(27)	1502(1)	2627(2)	731(1)	31(1)
C(28)	1038(1)	3057(2)	760(1)	35(1)
C(29)	1131(1)	3603(2)	1210(1)	36(1)
C(30)	1676(1)	3713(2)	1637(1)	28(1)
C(31)	2873(1)	4867(2)	2223(1)	19(1)
C(32)	2637(1)	5409(2)	1738(1)	34(1)
C(33)	2628(1)	6457(2)	1747(1)	42(1)
C(34)	2859(1)	6981(2)	2232(1)	35(1)
C(35)	3094(1)	6451(2)	2707(1)	26(1)

C(36)	3094(1)	5397(2)	2704(1)	20(1)
C(37)	4172(1)	4454(2)	3900(1)	17(1)
C(38)	4438(1)	5299(2)	3821(1)	24(1)
C(39)	4595(1)	6113(2)	4177(1)	30(1)
C(40)	4496(1)	6089(2)	4619(1)	29(1)
C(41)	4236(1)	5256(2)	4704(1)	27(1)
C(42)	4069(1)	4444(2)	4341(1)	23(1)
C(43)	4493(1)	2453(2)	3935(1)	15(1)
C(44)	4369(1)	1974(2)	4311(1)	19(1)
C(45)	4770(1)	1350(2)	4704(1)	21(1)
C(46)	5298(1)	1172(2)	4723(1)	24(1)
C(47)	5423(1)	1624(2)	4346(1)	23(1)
C(48)	5026(1)	2258(2)	3955(1)	20(1)
C(49)	572(1)	3179(2)	4241(1)	26(1)
C(50)	229(1)	2403(2)	4272(1)	29(1)
C(51)	-227(1)	2572(3)	4385(1)	39(1)
C(52)	-343(1)	3545(3)	4483(1)	47(1)
C(53)	-12(1)	4340(3)	4466(1)	46(1)
C(54)	447(1)	4152(2)	4357(1)	36(1)
C(55)	2310(1)	912(2)	4434(1)	18(1)
C(56)	2694(1)	224(2)	4391(1)	22(1)
C(57)	3145(1)	-172(2)	4847(1)	28(1)
C(58)	3235(1)	116(2)	5354(1)	33(1)
C(59)	2854(1)	770(2)	5405(1)	31(1)
C(60)	2393(1)	1152(2)	4949(1)	24(1)
C(61)	1479(1)	371(2)	3377(1)	20(1)
C(62)	1185(1)	-379(2)	3504(1)	26(1)
C(63)	962(1)	-1206(2)	3171(1)	31(1)
C(64)	1029(1)	-1307(2)	2712(1)	32(1)
C(65)	1329(1)	-584(2)	2589(1)	33(1)
C(66)	1554(1)	254(2)	2925(1)	24(1)
C(67)	723(1)	2396(2)	2544(1)	19(1)
C(68)	866(1)	2161(2)	2134(1)	24(1)
C(69)	536(1)	1488(2)	1730(1)	30(1)
C(70)	69(1)	1015(2)	1734(1)	36(1)
C(71)	-71(1)	1235(2)	2140(1)	30(1)
C(72)	249(1)	1922(2)	2536(1)	23(1)
C(73)	1045(1)	4442(2)	2614(1)	17(1)
C(74)	554(1)	4511(2)	2118(1)	23(1)
C(75)	440(1)	5370(2)	1799(1)	28(1)
C(76)	827(1)	6170(2)	1966(1)	28(1)
C(77)	1314(1)	6115(2)	2461(1)	24(1)
C(78)	1421(1)	5273(2)	2786(1)	19(1)
C(79)	2265(1)	5050(2)	4201(1)	18(1)
C(80)	2721(1)	5421(2)	4130(1)	23(1)
C(81)	2750(1)	6434(2)	4015(1)	28(1)
C(82)	2320(1)	7094(2)	3961(1)	30(1)
C(83)	1863(1)	6738(2)	4028(1)	29(1)
C(84)	1839(1)	5727(2)	4149(1)	23(1)
C(85)	2910(1)	3442(2)	4913(1)	19(1)
C(86)	3340(1)	2874(2)	4884(1)	22(1)
C(87)	3844(1)	2642(2)	5349(1)	25(1)
C(88)	3921(1)	2965(2)	5843(1)	29(1)
C(89)	3493(1)	3512(2)	5879(1)	33(1)

C(90)	2992(1)	3758(2)	5416(1)	29(1)
C(101)	3666(1)	7534(2)	1429(1)	39(1)
C(102)	3260(1)	7329(3)	914(1)	48(1)
C(103)	3190(2)	7953(3)	501(2)	56(1)
C(104)	3527(2)	8794(3)	597(2)	62(1)
C(105)	3939(1)	9025(3)	1124(2)	47(1)
C(106)	4009(1)	8387(2)	1539(1)	36(1)
C(111)	8885(2)	4569(3)	-7(2)	63(1)
C(112)	9426(2)	4238(3)	356(2)	60(1)
C(113)	9495(2)	3279(3)	557(2)	62(1)
C(114)	9042(2)	2636(3)	392(2)	59(1)
C(115)	8500(2)	2958(3)	26(2)	67(1)
C(116)	8422(2)	3925(3)	-168(2)	71(1)

Table 3. Selected bond lengths [Å] and angles [°] for MJA08 (CCDC 163590).

Co(1)-P(1)	2.2243(8)	Cl(1)-Co(1)-Cl(2)	80.65(2)
Co(1)-P(2)	2.2444(8)	Cl(1)-Co(2)-Cl(2)	79.79(2)
Co(1)-Cl(1)	2.2840(7)	Co(1)-Cl(1)-Co(2)	99.02(3)
Co(1)-Cl(2)	2.3206(7)	Co(1)-Cl(2)-Co(2)	97.46(3)
Co(1)-P(3)	2.3911(8)		
Co(2)-P(4)	2.2266(8)		
Co(2)-P(5)	2.2386(8)		
Co(2)-Cl(1)	2.3141(7)		
Co(2)-Cl(2)	2.3319(7)		
Co(2)-P(6)	2.3356(8)		

Table 4. Bond lengths [Å] and angles [°] for MJA08 (CCDC 163590).

Co(1)-P(1)	2.2243(8)	C(8)-H(8)	0.9500
Co(1)-P(2)	2.2444(8)	C(9)-C(10)	1.386(4)
Co(1)-Cl(1)	2.2840(7)	C(9)-H(9)	0.9500
Co(1)-Cl(2)	2.3206(7)	C(10)-C(11)	1.388(4)
Co(1)-P(3)	2.3911(8)	C(10)-H(10)	0.9500
Co(2)-P(4)	2.2266(8)	C(11)-C(12)	1.393(3)
Co(2)-P(5)	2.2386(8)	C(11)-H(11)	0.9500
Co(2)-Cl(1)	2.3141(7)	C(12)-H(12)	0.9500
Co(2)-Cl(2)	2.3319(7)	C(13)-C(14)	1.393(3)
Co(2)-P(6)	2.3356(8)	C(13)-C(18)	1.408(3)
P(1)-C(1)	1.807(2)	C(14)-C(15)	1.386(3)
P(1)-C(13)	1.836(3)	C(14)-H(14)	0.9500
P(1)-C(19)	1.836(3)	C(15)-C(16)	1.385(3)
P(2)-C(2)	1.821(2)	C(15)-H(15)	0.9500
P(2)-C(25)	1.835(3)	C(16)-C(17)	1.386(3)
P(2)-C(31)	1.855(3)	C(16)-H(16)	0.9500
P(3)-C(3)	1.802(2)	C(17)-C(18)	1.380(3)
P(3)-C(43)	1.839(2)	C(17)-H(17)	0.9500
P(3)-C(37)	1.855(3)	C(18)-H(18)	0.9500
P(4)-C(4)	1.820(2)	C(19)-C(24)	1.392(3)
P(4)-C(61)	1.836(3)	C(19)-C(20)	1.396(3)
P(4)-C(55)	1.836(3)	C(20)-C(21)	1.383(4)
P(5)-C(5)	1.811(2)	C(20)-H(20)	0.9500
P(5)-C(67)	1.818(3)	C(21)-C(22)	1.378(4)
P(5)-C(73)	1.851(3)	C(21)-H(21)	0.9500
P(6)-C(6)	1.830(2)	C(22)-C(23)	1.382(4)
P(6)-C(85)	1.838(3)	C(22)-H(22)	0.9500
P(6)-C(79)	1.840(3)	C(23)-C(24)	1.395(4)
B(1)-C(7)	1.632(4)	C(23)-H(23)	0.9500
B(1)-C(2)	1.655(4)	C(24)-H(24)	0.9500
B(1)-C(1)	1.663(4)	C(25)-C(26)	1.397(3)
B(1)-C(3)	1.671(4)	C(25)-C(30)	1.399(3)
B(2)-C(6)	1.644(4)	C(26)-C(27)	1.383(3)
B(2)-C(49)	1.643(4)	C(26)-H(26)	0.9500
B(2)-C(4)	1.656(4)	C(27)-C(28)	1.382(4)
B(2)-C(5)	1.666(4)	C(27)-H(27)	0.9500
C(1)-H(1A)	0.9900	C(28)-C(29)	1.372(4)
C(1)-H(1B)	0.9900	C(28)-H(28)	0.9500
C(2)-H(2A)	0.9900	C(29)-C(30)	1.380(3)
C(2)-H(2B)	0.9900	C(29)-H(29)	0.9500
C(3)-H(3A)	0.9900	C(30)-H(30)	0.9500
C(3)-H(3B)	0.9900	C(31)-C(36)	1.382(3)
C(4)-H(4A)	0.9900	C(31)-C(32)	1.398(4)
C(4)-H(4B)	0.9900	C(32)-C(33)	1.385(4)
C(5)-H(5A)	0.9900	C(32)-H(32)	0.9500
C(5)-H(5B)	0.9900	C(33)-C(34)	1.387(4)
C(6)-H(6A)	0.9900	C(33)-H(33)	0.9500
C(6)-H(6B)	0.9900	C(34)-C(35)	1.369(4)
C(7)-C(12)	1.403(3)	C(34)-H(34)	0.9500
C(7)-C(8)	1.408(3)	C(35)-C(36)	1.393(3)
C(8)-C(9)	1.389(3)	C(35)-H(35)	0.9500

C(36)-H(36)	0.9500	C(65)-H(65)	0.9500
C(37)-C(42)	1.383(3)	C(66)-H(66)	0.9500
C(37)-C(38)	1.391(3)	C(67)-C(72)	1.388(3)
C(38)-C(39)	1.390(3)	C(67)-C(68)	1.401(3)
C(38)-H(38)	0.9500	C(68)-C(69)	1.381(3)
C(39)-C(40)	1.382(4)	C(68)-H(68)	0.9500
C(39)-H(39)	0.9500	C(69)-C(70)	1.386(4)
C(40)-C(41)	1.374(4)	C(69)-H(69)	0.9500
C(40)-H(40)	0.9500	C(70)-C(71)	1.381(4)
C(41)-C(42)	1.400(3)	C(70)-H(70)	0.9500
C(41)-H(41)	0.9500	C(71)-C(72)	1.375(4)
C(42)-H(42)	0.9500	C(71)-H(71)	0.9500
C(43)-C(44)	1.393(3)	C(72)-H(72)	0.9500
C(43)-C(48)	1.402(3)	C(73)-C(74)	1.390(3)
C(44)-C(45)	1.386(3)	C(73)-C(78)	1.403(3)
C(44)-H(44)	0.9500	C(74)-C(75)	1.389(3)
C(45)-C(46)	1.387(3)	C(74)-H(74)	0.9500
C(45)-H(45)	0.9500	C(75)-C(76)	1.388(4)
C(46)-C(47)	1.378(3)	C(75)-H(75)	0.9500
C(46)-H(46)	0.9500	C(76)-C(77)	1.381(3)
C(47)-C(48)	1.387(3)	C(76)-H(76)	0.9500
C(47)-H(47)	0.9500	C(77)-C(78)	1.383(3)
C(48)-H(48)	0.9500	C(77)-H(77)	0.9500
C(49)-C(50)	1.395(4)	C(78)-H(78)	0.9500
C(49)-C(54)	1.403(4)	C(79)-C(84)	1.389(3)
C(50)-C(51)	1.398(4)	C(79)-C(80)	1.394(3)
C(50)-H(50)	0.9500	C(80)-C(81)	1.387(3)
C(51)-C(52)	1.377(4)	C(80)-H(80)	0.9500
C(51)-H(51)	0.9500	C(81)-C(82)	1.379(4)
C(52)-C(53)	1.380(4)	C(81)-H(81)	0.9500
C(52)-H(52)	0.9500	C(82)-C(83)	1.385(4)
C(53)-C(54)	1.403(4)	C(82)-H(82)	0.9500
C(53)-H(53)	0.9500	C(83)-C(84)	1.386(3)
C(54)-H(54)	0.9500	C(83)-H(83)	0.9500
C(55)-C(60)	1.389(3)	C(84)-H(84)	0.9500
C(55)-C(56)	1.406(3)	C(85)-C(90)	1.386(3)
C(56)-C(57)	1.378(3)	C(85)-C(86)	1.392(3)
C(56)-H(56)	0.9500	C(86)-C(87)	1.391(3)
C(57)-C(58)	1.379(4)	C(86)-H(86)	0.9500
C(57)-H(57)	0.9500	C(87)-C(88)	1.371(3)
C(58)-C(59)	1.381(4)	C(87)-H(87)	0.9500
C(58)-H(58)	0.9500	C(88)-C(89)	1.380(4)
C(59)-C(60)	1.382(4)	C(88)-H(88)	0.9500
C(59)-H(59)	0.9500	C(89)-C(90)	1.389(4)
C(60)-H(60)	0.9500	C(89)-H(89)	0.9500
C(61)-C(66)	1.379(3)	C(90)-H(90)	0.9500
C(61)-C(62)	1.402(3)	C(101)-C(102)	1.362(4)
C(62)-C(63)	1.377(4)	C(101)-C(106)	1.385(4)
C(62)-H(62)	0.9500	C(101)-H(101)	0.9500
C(63)-C(64)	1.386(4)	C(102)-C(103)	1.362(4)
C(63)-H(63)	0.9500	C(102)-H(102)	0.9500
C(64)-C(65)	1.382(4)	C(103)-C(104)	1.369(5)
C(64)-H(64)	0.9500	C(103)-H(103)	0.9500
C(65)-C(66)	1.393(4)	C(104)-C(105)	1.395(5)

C(104)-H(104)	0.9500	C(3)-P(3)-Co(1)	108.18(8)
C(105)-C(106)	1.378(4)	C(43)-P(3)-Co(1)	115.13(8)
C(105)-H(105)	0.9500	C(37)-P(3)-Co(1)	123.91(8)
C(106)-H(106)	0.9500	C(4)-P(4)-C(61)	104.99(12)
C(111)-C(112)	1.378(5)	C(4)-P(4)-C(55)	106.28(12)
C(111)-C(116)	1.378(5)	C(61)-P(4)-C(55)	100.78(12)
C(111)-H(111)	0.9500	C(4)-P(4)-Co(2)	115.33(8)
C(112)-C(113)	1.365(5)	C(61)-P(4)-Co(2)	116.42(9)
C(112)-H(112)	0.9500	C(55)-P(4)-Co(2)	111.59(8)
C(113)-C(114)	1.358(5)	C(5)-P(5)-C(67)	108.04(12)
C(113)-H(113)	0.9500	C(5)-P(5)-C(73)	104.24(11)
C(114)-C(115)	1.380(4)	C(67)-P(5)-C(73)	100.13(12)
C(114)-H(114)	0.9500	C(5)-P(5)-Co(2)	113.49(9)
C(115)-C(116)	1.366(5)	C(67)-P(5)-Co(2)	111.51(8)
C(115)-H(115)	0.9500	C(73)-P(5)-Co(2)	118.20(9)
C(116)-H(116)	0.9500	C(6)-P(6)-C(85)	104.27(12)
		C(6)-P(6)-C(79)	104.61(12)
P(1)-Co(1)-P(2)	88.16(3)	C(85)-P(6)-C(79)	102.38(12)
P(1)-Co(1)-Cl(1)	162.76(3)	C(6)-P(6)-Co(2)	114.40(9)
P(2)-Co(1)-Cl(1)	92.82(3)	C(85)-P(6)-Co(2)	117.27(9)
P(1)-Co(1)-Cl(2)	92.55(3)	C(79)-P(6)-Co(2)	112.44(9)
P(2)-Co(1)-Cl(2)	159.70(3)	C(7)-B(1)-C(2)	110.6(2)
Cl(1)-Co(1)-Cl(2)	80.65(2)	C(7)-B(1)-C(1)	109.4(2)
P(1)-Co(1)-P(3)	91.09(3)	C(2)-B(1)-C(1)	108.0(2)
P(2)-Co(1)-P(3)	92.66(3)	C(7)-B(1)-C(3)	106.5(2)
Cl(1)-Co(1)-P(3)	106.04(3)	C(2)-B(1)-C(3)	109.0(2)
Cl(2)-Co(1)-P(3)	107.60(3)	C(1)-B(1)-C(3)	113.4(2)
P(4)-Co(2)-P(5)	88.69(3)	C(6)-B(2)-C(49)	109.6(2)
P(4)-Co(2)-Cl(1)	168.14(3)	C(6)-B(2)-C(4)	109.6(2)
P(5)-Co(2)-Cl(1)	94.20(3)	C(49)-B(2)-C(4)	110.4(2)
P(4)-Co(2)-Cl(2)	91.74(3)	C(6)-B(2)-C(5)	111.0(2)
P(5)-Co(2)-Cl(2)	148.38(3)	C(49)-B(2)-C(5)	106.1(2)
Cl(1)-Co(2)-Cl(2)	79.79(2)	C(4)-B(2)-C(5)	110.1(2)
P(4)-Co(2)-P(6)	89.08(3)	B(1)-C(1)-P(1)	115.49(17)
P(5)-Co(2)-P(6)	93.53(3)	B(1)-C(1)-H(1A)	108.4
Cl(1)-Co(2)-P(6)	102.19(3)	P(1)-C(1)-H(1A)	108.4
Cl(2)-Co(2)-P(6)	118.09(3)	B(1)-C(1)-H(1B)	108.4
Co(1)-Cl(1)-Co(2)	99.02(3)	P(1)-C(1)-H(1B)	108.4
Co(1)-Cl(2)-Co(2)	97.46(3)	H(1A)-C(1)-H(1B)	107.5
C(1)-P(1)-C(13)	107.34(12)	B(1)-C(2)-P(2)	114.05(17)
C(1)-P(1)-C(19)	107.37(12)	B(1)-C(2)-H(2A)	108.7
C(13)-P(1)-C(19)	98.24(12)	P(2)-C(2)-H(2A)	108.7
C(1)-P(1)-Co(1)	112.89(9)	B(1)-C(2)-H(2B)	108.7
C(13)-P(1)-Co(1)	114.44(8)	P(2)-C(2)-H(2B)	108.7
C(19)-P(1)-Co(1)	115.32(9)	H(2A)-C(2)-H(2B)	107.6
C(2)-P(2)-C(25)	107.30(12)	B(1)-C(3)-P(3)	115.19(17)
C(2)-P(2)-C(31)	105.34(12)	B(1)-C(3)-H(3A)	108.5
C(25)-P(2)-C(31)	99.20(12)	P(3)-C(3)-H(3A)	108.5
C(2)-P(2)-Co(1)	114.29(9)	B(1)-C(3)-H(3B)	108.5
C(25)-P(2)-Co(1)	115.01(9)	P(3)-C(3)-H(3B)	108.5
C(31)-P(2)-Co(1)	114.23(9)	H(3A)-C(3)-H(3B)	107.5
C(3)-P(3)-C(43)	105.27(11)	B(2)-C(4)-P(4)	116.92(17)
C(3)-P(3)-C(37)	105.68(12)	B(2)-C(4)-H(4A)	108.1
C(43)-P(3)-C(37)	96.85(11)	P(4)-C(4)-H(4A)	108.1

B(2)-C(4)-H(4B)	108.1	C(21)-C(20)-C(19)	121.3(3)
P(4)-C(4)-H(4B)	108.1	C(21)-C(20)-H(20)	119.4
H(4A)-C(4)-H(4B)	107.3	C(19)-C(20)-H(20)	119.4
B(2)-C(5)-P(5)	117.12(17)	C(22)-C(21)-C(20)	119.8(3)
B(2)-C(5)-H(5A)	108.0	C(22)-C(21)-H(21)	120.1
P(5)-C(5)-H(5A)	108.0	C(20)-C(21)-H(21)	120.1
B(2)-C(5)-H(5B)	108.0	C(23)-C(22)-C(21)	120.3(3)
P(5)-C(5)-H(5B)	108.0	C(23)-C(22)-H(22)	119.8
H(5A)-C(5)-H(5B)	107.3	C(21)-C(22)-H(22)	119.8
B(2)-C(6)-P(6)	115.61(18)	C(22)-C(23)-C(24)	119.8(3)
B(2)-C(6)-H(6A)	108.4	C(22)-C(23)-H(23)	120.1
P(6)-C(6)-H(6A)	108.4	C(24)-C(23)-H(23)	120.1
B(2)-C(6)-H(6B)	108.4	C(19)-C(24)-C(23)	120.7(3)
P(6)-C(6)-H(6B)	108.4	C(19)-C(24)-H(24)	119.7
H(6A)-C(6)-H(6B)	107.4	C(23)-C(24)-H(24)	119.7
C(12)-C(7)-C(8)	114.7(2)	C(26)-C(25)-C(30)	117.7(2)
C(12)-C(7)-B(1)	124.1(2)	C(26)-C(25)-P(2)	123.6(2)
C(8)-C(7)-B(1)	121.0(2)	C(30)-C(25)-P(2)	118.7(2)
C(9)-C(8)-C(7)	123.1(3)	C(27)-C(26)-C(25)	121.0(3)
C(9)-C(8)-H(8)	118.5	C(27)-C(26)-H(26)	119.5
C(7)-C(8)-H(8)	118.5	C(25)-C(26)-H(26)	119.5
C(10)-C(9)-C(8)	120.3(3)	C(28)-C(27)-C(26)	120.3(3)
C(10)-C(9)-H(9)	119.8	C(28)-C(27)-H(27)	119.8
C(8)-C(9)-H(9)	119.8	C(26)-C(27)-H(27)	119.8
C(9)-C(10)-C(11)	118.7(3)	C(29)-C(28)-C(27)	119.2(3)
C(9)-C(10)-H(10)	120.7	C(29)-C(28)-H(28)	120.4
C(11)-C(10)-H(10)	120.7	C(27)-C(28)-H(28)	120.4
C(10)-C(11)-C(12)	120.2(3)	C(28)-C(29)-C(30)	121.2(3)
C(10)-C(11)-H(11)	119.9	C(28)-C(29)-H(29)	119.4
C(12)-C(11)-H(11)	119.9	C(30)-C(29)-H(29)	119.4
C(11)-C(12)-C(7)	123.1(3)	C(29)-C(30)-C(25)	120.5(3)
C(11)-C(12)-H(12)	118.5	C(29)-C(30)-H(30)	119.7
C(7)-C(12)-H(12)	118.5	C(25)-C(30)-H(30)	119.7
C(14)-C(13)-C(18)	117.5(2)	C(36)-C(31)-C(32)	118.7(3)
C(14)-C(13)-P(1)	122.5(2)	C(36)-C(31)-P(2)	122.8(2)
C(18)-C(13)-P(1)	120.0(2)	C(32)-C(31)-P(2)	118.5(2)
C(15)-C(14)-C(13)	121.1(3)	C(33)-C(32)-C(31)	119.9(3)
C(15)-C(14)-H(14)	119.5	C(33)-C(32)-H(32)	120.1
C(13)-C(14)-H(14)	119.5	C(31)-C(32)-H(32)	120.1
C(16)-C(15)-C(14)	120.4(3)	C(34)-C(33)-C(32)	120.9(3)
C(16)-C(15)-H(15)	119.8	C(34)-C(33)-H(33)	119.5
C(14)-C(15)-H(15)	119.8	C(32)-C(33)-H(33)	119.5
C(15)-C(16)-C(17)	119.7(3)	C(35)-C(34)-C(33)	119.2(3)
C(15)-C(16)-H(16)	120.1	C(35)-C(34)-H(34)	120.4
C(17)-C(16)-H(16)	120.1	C(33)-C(34)-H(34)	120.4
C(18)-C(17)-C(16)	119.7(3)	C(34)-C(35)-C(36)	120.5(3)
C(18)-C(17)-H(17)	120.1	C(34)-C(35)-H(35)	119.7
C(16)-C(17)-H(17)	120.1	C(36)-C(35)-H(35)	119.7
C(17)-C(18)-C(13)	121.6(3)	C(31)-C(36)-C(35)	120.7(3)
C(17)-C(18)-H(18)	119.2	C(31)-C(36)-H(36)	119.6
C(13)-C(18)-H(18)	119.2	C(35)-C(36)-H(36)	119.6
C(24)-C(19)-C(20)	118.1(3)	C(42)-C(37)-C(38)	118.2(2)
C(24)-C(19)-P(1)	120.0(2)	C(42)-C(37)-P(3)	119.4(2)
C(20)-C(19)-P(1)	121.3(2)	C(38)-C(37)-P(3)	122.3(2)

C(39)-C(38)-C(37)	120.8(3)	C(57)-C(56)-C(55)	120.6(3)
C(39)-C(38)-H(38)	119.6	C(57)-C(56)-H(56)	119.7
C(37)-C(38)-H(38)	119.6	C(55)-C(56)-H(56)	119.7
C(40)-C(39)-C(38)	120.4(3)	C(58)-C(57)-C(56)	120.5(3)
C(40)-C(39)-H(39)	119.8	C(58)-C(57)-H(57)	119.8
C(38)-C(39)-H(39)	119.8	C(56)-C(57)-H(57)	119.8
C(41)-C(40)-C(39)	119.5(3)	C(57)-C(58)-C(59)	119.8(3)
C(41)-C(40)-H(40)	120.3	C(57)-C(58)-H(58)	120.1
C(39)-C(40)-H(40)	120.3	C(59)-C(58)-H(58)	120.1
C(40)-C(41)-C(42)	120.1(3)	C(58)-C(59)-C(60)	119.9(3)
C(40)-C(41)-H(41)	119.9	C(58)-C(59)-H(59)	120.0
C(42)-C(41)-H(41)	119.9	C(60)-C(59)-H(59)	120.0
C(37)-C(42)-C(41)	121.0(3)	C(59)-C(60)-C(55)	121.3(3)
C(37)-C(42)-H(42)	119.5	C(59)-C(60)-H(60)	119.3
C(41)-C(42)-H(42)	119.5	C(55)-C(60)-H(60)	119.3
C(44)-C(43)-C(48)	118.2(2)	C(66)-C(61)-C(62)	119.0(3)
C(44)-C(43)-P(3)	119.46(19)	C(66)-C(61)-P(4)	122.6(2)
C(48)-C(43)-P(3)	122.35(19)	C(62)-C(61)-P(4)	118.3(2)
C(45)-C(44)-C(43)	120.6(2)	C(63)-C(62)-C(61)	120.2(3)
C(45)-C(44)-H(44)	119.7	C(63)-C(62)-H(62)	119.9
C(43)-C(44)-H(44)	119.7	C(61)-C(62)-H(62)	119.9
C(46)-C(45)-C(44)	120.6(2)	C(62)-C(63)-C(64)	120.3(3)
C(46)-C(45)-H(45)	119.7	C(62)-C(63)-H(63)	119.9
C(44)-C(45)-H(45)	119.7	C(64)-C(63)-H(63)	119.9
C(47)-C(46)-C(45)	119.4(3)	C(63)-C(64)-C(65)	120.1(3)
C(47)-C(46)-H(46)	120.3	C(63)-C(64)-H(64)	120.0
C(45)-C(46)-H(46)	120.3	C(65)-C(64)-H(64)	120.0
C(46)-C(47)-C(48)	120.4(2)	C(64)-C(65)-C(66)	119.6(3)
C(46)-C(47)-H(47)	119.8	C(64)-C(65)-H(65)	120.2
C(48)-C(47)-H(47)	119.8	C(66)-C(65)-H(65)	120.2
C(47)-C(48)-C(43)	120.8(2)	C(61)-C(66)-C(65)	120.8(3)
C(47)-C(48)-H(48)	119.6	C(61)-C(66)-H(66)	119.6
C(43)-C(48)-H(48)	119.6	C(65)-C(66)-H(66)	119.6
C(50)-C(49)-C(54)	115.5(3)	C(72)-C(67)-C(68)	118.1(2)
C(50)-C(49)-B(2)	124.7(3)	C(72)-C(67)-P(5)	124.6(2)
C(54)-C(49)-B(2)	119.7(3)	C(68)-C(67)-P(5)	117.27(19)
C(49)-C(50)-C(51)	123.2(3)	C(69)-C(68)-C(67)	120.6(3)
C(49)-C(50)-H(50)	118.4	C(69)-C(68)-H(68)	119.7
C(51)-C(50)-H(50)	118.4	C(67)-C(68)-H(68)	119.7
C(52)-C(51)-C(50)	119.2(3)	C(68)-C(69)-C(70)	120.1(3)
C(52)-C(51)-H(51)	120.4	C(68)-C(69)-H(69)	119.9
C(50)-C(51)-H(51)	120.4	C(70)-C(69)-H(69)	119.9
C(51)-C(52)-C(53)	120.1(3)	C(71)-C(70)-C(69)	119.5(3)
C(51)-C(52)-H(52)	119.9	C(71)-C(70)-H(70)	120.2
C(53)-C(52)-H(52)	119.9	C(69)-C(70)-H(70)	120.2
C(52)-C(53)-C(54)	119.7(3)	C(72)-C(71)-C(70)	120.3(3)
C(52)-C(53)-H(53)	120.1	C(72)-C(71)-H(71)	119.8
C(54)-C(53)-H(53)	120.1	C(70)-C(71)-H(71)	119.8
C(53)-C(54)-C(49)	122.2(3)	C(71)-C(72)-C(67)	121.2(3)
C(53)-C(54)-H(54)	118.9	C(71)-C(72)-H(72)	119.4
C(49)-C(54)-H(54)	118.9	C(67)-C(72)-H(72)	119.4
C(60)-C(55)-C(56)	117.8(2)	C(74)-C(73)-C(78)	118.0(2)
C(60)-C(55)-P(4)	122.9(2)	C(74)-C(73)-P(5)	120.4(2)
C(56)-C(55)-P(4)	119.3(2)	C(78)-C(73)-P(5)	121.4(2)

C(73)-C(74)-C(75)	121.1(3)	C(103)-C(102)-C(101)	120.4(4)
C(73)-C(74)-H(74)	119.5	C(103)-C(102)-H(102)	119.8
C(75)-C(74)-H(74)	119.5	C(101)-C(102)-H(102)	119.8
C(76)-C(75)-C(74)	120.1(3)	C(102)-C(103)-C(104)	120.4(4)
C(76)-C(75)-H(75)	119.9	C(102)-C(103)-H(103)	119.8
C(74)-C(75)-H(75)	119.9	C(104)-C(103)-H(103)	119.8
C(77)-C(76)-C(75)	119.4(3)	C(103)-C(104)-C(105)	119.9(4)
C(77)-C(76)-H(76)	120.3	C(103)-C(104)-H(104)	120.1
C(75)-C(76)-H(76)	120.3	C(105)-C(104)-H(104)	120.1
C(76)-C(77)-C(78)	120.6(3)	C(106)-C(105)-C(104)	119.3(4)
C(76)-C(77)-H(77)	119.7	C(106)-C(105)-H(105)	120.3
C(78)-C(77)-H(77)	119.7	C(104)-C(105)-H(105)	120.3
C(77)-C(78)-C(73)	120.7(2)	C(105)-C(106)-C(101)	119.6(3)
C(77)-C(78)-H(78)	119.7	C(105)-C(106)-H(106)	120.2
C(73)-C(78)-H(78)	119.7	C(101)-C(106)-H(106)	120.2
C(84)-C(79)-C(80)	117.7(2)	C(112)-C(111)-C(116)	119.8(4)
C(84)-C(79)-P(6)	124.2(2)	C(112)-C(111)-H(111)	120.1
C(80)-C(79)-P(6)	117.8(2)	C(116)-C(111)-H(111)	120.1
C(81)-C(80)-C(79)	121.2(3)	C(113)-C(112)-C(111)	119.4(4)
C(81)-C(80)-H(80)	119.4	C(113)-C(112)-H(112)	120.3
C(79)-C(80)-H(80)	119.4	C(111)-C(112)-H(112)	120.3
C(82)-C(81)-C(80)	120.2(3)	C(112)-C(113)-C(114)	121.0(4)
C(82)-C(81)-H(81)	119.9	C(112)-C(113)-H(113)	119.5
C(80)-C(81)-H(81)	119.9	C(114)-C(113)-H(113)	119.5
C(81)-C(82)-C(83)	119.4(3)	C(113)-C(114)-C(115)	119.9(4)
C(81)-C(82)-H(82)	120.3	C(113)-C(114)-H(114)	120.0
C(83)-C(82)-H(82)	120.3	C(115)-C(114)-H(114)	120.0
C(84)-C(83)-C(82)	120.1(3)	C(116)-C(115)-C(114)	119.6(4)
C(84)-C(83)-H(83)	120.0	C(116)-C(115)-H(115)	120.2
C(82)-C(83)-H(83)	120.0	C(114)-C(115)-H(115)	120.2
C(83)-C(84)-C(79)	121.3(3)	C(115)-C(116)-C(111)	120.2(4)
C(83)-C(84)-H(84)	119.3	C(115)-C(116)-H(116)	119.9
C(79)-C(84)-H(84)	119.3	C(111)-C(116)-H(116)	119.9
C(90)-C(85)-C(86)	118.5(2)		
C(90)-C(85)-P(6)	121.9(2)		
C(86)-C(85)-P(6)	119.4(2)		
C(85)-C(86)-C(87)	120.7(3)		
C(85)-C(86)-H(86)	119.6		
C(87)-C(86)-H(86)	119.6		
C(88)-C(87)-C(86)	120.0(3)		
C(88)-C(87)-H(87)	120.0		
C(86)-C(87)-H(87)	120.0		
C(87)-C(88)-C(89)	119.9(3)		
C(87)-C(88)-H(88)	120.1		
C(89)-C(88)-H(88)	120.1		
C(88)-C(89)-C(90)	120.4(3)		
C(88)-C(89)-H(89)	119.8		
C(90)-C(89)-H(89)	119.8		
C(85)-C(90)-C(89)	120.4(3)		
C(85)-C(90)-H(90)	119.8		
C(89)-C(90)-H(90)	119.8		
C(102)-C(101)-C(106)	120.4(3)		
C(102)-C(101)-H(101)	119.8		
C(106)-C(101)-H(101)	119.8		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for MJA08 (CCDC 163590). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	152(2)	162(2)	169(2)	-1(2)	85(2)	1(2)
Co(2)	140(2)	161(2)	187(2)	7(2)	88(2)	5(2)
Cl(1)	216(4)	184(3)	253(4)	33(3)	151(3)	34(3)
Cl(2)	180(3)	182(3)	208(4)	13(3)	114(3)	18(3)
P(1)	165(4)	177(4)	194(4)	-10(3)	100(3)	-10(3)
P(2)	163(4)	206(4)	168(4)	4(3)	79(3)	4(3)
P(3)	153(4)	165(4)	164(4)	1(3)	73(3)	1(3)
P(4)	161(4)	175(4)	220(4)	12(3)	103(3)	2(3)
P(5)	150(4)	178(4)	205(4)	4(3)	86(3)	3(3)
P(6)	186(4)	193(4)	172(4)	9(3)	90(3)	8(3)
B(1)	165(16)	210(17)	168(18)	9(14)	101(14)	9(14)
B(2)	193(17)	221(18)	220(20)	60(14)	113(16)	62(14)
C(1)	152(14)	226(15)	205(16)	-22(12)	116(13)	26(11)
C(2)	207(15)	248(16)	183(16)	-5(12)	132(13)	-8(12)
C(3)	150(14)	178(15)	184(16)	65(12)	81(12)	18(11)
C(4)	159(14)	255(16)	210(16)	46(13)	102(13)	-8(12)
C(5)	170(14)	201(15)	268(17)	-35(13)	133(13)	5(12)
C(6)	252(16)	201(15)	230(16)	61(13)	159(14)	82(12)
C(7)	182(14)	259(16)	115(15)	-39(12)	56(12)	-27(12)
C(8)	264(16)	272(17)	286(18)	2(14)	158(15)	12(13)
C(9)	296(18)	354(19)	360(20)	55(15)	206(16)	-71(14)
C(10)	231(17)	490(20)	247(18)	-23(15)	172(15)	-36(15)
C(11)	161(15)	326(18)	214(17)	-64(13)	81(13)	-5(12)
C(12)	218(15)	254(17)	217(17)	-19(13)	123(14)	-46(12)
C(13)	232(16)	138(14)	200(16)	-39(12)	144(13)	28(12)
C(14)	269(17)	199(16)	250(17)	-25(13)	144(15)	-19(13)
C(15)	269(17)	217(16)	235(18)	-28(13)	107(14)	29(13)
C(16)	377(18)	163(15)	234(17)	19(13)	176(15)	31(13)
C(17)	300(17)	178(15)	340(19)	-18(14)	209(16)	-41(13)
C(18)	188(15)	217(16)	251(18)	18(13)	113(14)	14(12)
C(19)	198(15)	203(15)	221(17)	10(13)	115(14)	-28(12)
C(20)	217(16)	270(17)	300(18)	-48(14)	144(15)	-37(13)
C(21)	325(19)	360(19)	306(19)	-132(15)	184(16)	-85(15)
C(22)	312(19)	400(20)	330(20)	-133(16)	107(17)	-128(15)
C(23)	184(16)	390(20)	330(20)	-52(16)	66(15)	-55(14)
C(24)	247(16)	258(16)	279(18)	-40(14)	156(15)	-15(13)
C(25)	146(14)	281(16)	139(16)	38(13)	37(13)	-17(12)
C(26)	206(15)	322(17)	240(18)	9(14)	100(14)	9(13)
C(27)	278(17)	440(20)	219(18)	-89(15)	114(15)	-79(15)
C(28)	172(16)	640(20)	196(18)	-27(16)	57(14)	-45(15)
C(29)	170(16)	680(20)	226(18)	5(17)	92(14)	55(16)
C(30)	204(16)	427(19)	189(17)	-22(14)	80(14)	-11(14)
C(31)	230(15)	196(15)	197(16)	35(13)	138(14)	13(12)
C(32)	480(20)	279(18)	274(19)	27(15)	185(17)	-18(15)
C(33)	630(20)	299(19)	310(20)	143(16)	203(19)	56(17)
C(34)	470(20)	186(17)	400(20)	47(15)	218(18)	-4(14)
C(35)	295(17)	222(16)	274(18)	-9(14)	133(15)	-15(13)

C(36)	152(14)	223(16)	235(17)	47(13)	95(13)	16(12)
C(37)	139(14)	175(15)	168(16)	5(12)	38(12)	36(11)
C(38)	256(16)	234(16)	223(17)	-6(13)	111(14)	4(13)
C(39)	278(17)	197(16)	360(20)	-25(14)	101(16)	-41(13)
C(40)	222(16)	250(17)	288(19)	-116(14)	27(15)	46(13)
C(41)	265(17)	309(18)	237(18)	-34(14)	109(14)	63(14)
C(42)	216(16)	232(16)	234(17)	4(13)	94(14)	12(12)
C(43)	143(13)	135(14)	130(15)	-26(11)	35(12)	-13(11)
C(44)	160(14)	182(15)	217(17)	-23(12)	90(13)	-5(11)
C(45)	236(16)	186(15)	198(16)	30(13)	93(14)	-31(12)
C(46)	191(15)	214(16)	240(18)	33(13)	32(14)	33(12)
C(47)	147(14)	237(16)	296(18)	47(14)	83(14)	58(12)
C(48)	200(15)	189(15)	218(16)	52(13)	108(13)	8(12)
C(49)	249(16)	344(18)	194(17)	72(14)	117(14)	89(14)
C(50)	208(16)	460(20)	214(17)	-57(15)	107(14)	-26(14)
C(51)	335(19)	590(20)	310(20)	-48(18)	201(16)	-94(17)
C(52)	310(20)	740(30)	490(20)	90(20)	289(19)	104(19)
C(53)	520(20)	540(20)	440(20)	97(18)	330(20)	244(19)
C(54)	342(19)	450(20)	330(20)	76(16)	196(17)	115(16)
C(55)	191(15)	157(14)	221(17)	39(12)	126(13)	-15(11)
C(56)	242(16)	211(15)	209(17)	30(13)	113(14)	-17(12)
C(57)	253(17)	253(17)	350(20)	79(15)	140(16)	92(13)
C(58)	279(18)	307(19)	310(20)	120(15)	71(16)	59(14)
C(59)	390(19)	286(18)	239(18)	53(14)	147(16)	19(15)
C(60)	223(16)	258(17)	252(18)	23(14)	125(14)	30(13)
C(61)	139(14)	189(15)	251(17)	21(13)	71(13)	44(12)
C(62)	230(16)	199(16)	312(19)	26(14)	100(15)	-5(13)
C(63)	186(16)	230(17)	450(20)	35(15)	104(16)	-3(13)
C(64)	192(16)	205(17)	430(20)	-96(15)	26(15)	4(13)
C(65)	268(18)	330(19)	370(20)	-111(16)	129(16)	-30(14)
C(66)	196(15)	197(16)	329(19)	-24(14)	117(14)	21(12)
C(67)	147(14)	154(14)	235(17)	0(12)	67(13)	31(11)
C(68)	201(15)	223(16)	298(18)	-27(14)	118(14)	-4(13)
C(69)	301(18)	304(18)	277(18)	-71(14)	131(15)	1(14)
C(70)	337(19)	291(18)	340(20)	-65(15)	71(17)	-111(14)
C(71)	245(17)	306(18)	320(20)	13(15)	99(15)	-78(14)
C(72)	193(15)	256(16)	248(17)	9(13)	108(14)	-15(12)
C(73)	200(15)	165(14)	174(16)	-2(12)	112(13)	52(12)
C(74)	243(16)	180(15)	233(17)	-38(13)	88(14)	-4(12)
C(75)	283(17)	276(18)	197(17)	9(14)	48(14)	74(14)
C(76)	376(19)	200(16)	221(18)	30(13)	112(15)	43(14)
C(77)	280(17)	190(16)	254(18)	0(13)	128(15)	6(13)
C(78)	165(14)	203(15)	162(16)	11(12)	48(12)	51(12)
C(79)	240(16)	181(15)	125(15)	-20(12)	84(13)	-4(12)
C(80)	243(16)	261(16)	171(16)	-18(13)	94(14)	9(13)
C(81)	342(18)	252(17)	278(18)	10(14)	172(15)	-76(14)
C(82)	460(20)	191(16)	251(18)	21(13)	170(16)	-2(14)
C(83)	392(19)	228(17)	268(18)	21(14)	179(16)	57(14)
C(84)	270(16)	222(16)	202(17)	-21(13)	115(14)	-34(13)
C(85)	209(15)	201(15)	152(16)	20(12)	76(13)	-26(12)
C(86)	245(16)	244(16)	157(16)	1(13)	89(13)	-23(13)
C(87)	234(16)	314(17)	194(17)	18(14)	90(14)	50(13)
C(88)	249(17)	390(20)	181(17)	79(14)	52(14)	2(14)
C(89)	351(19)	450(20)	141(17)	-1(15)	86(15)	-14(16)

C(90)	283(17)	336(18)	269(18)	-37(15)	137(15)	40(14)
C(101)	320(19)	450(20)	350(20)	74(17)	123(17)	86(16)
C(102)	350(20)	610(30)	430(20)	-100(20)	139(19)	114(18)
C(103)	360(20)	1010(40)	310(20)	-50(20)	153(19)	270(20)
C(104)	500(30)	1010(40)	480(30)	360(30)	360(20)	400(20)
C(105)	360(20)	560(20)	570(30)	190(20)	280(20)	184(18)
C(106)	281(18)	490(20)	310(20)	88(17)	145(16)	153(16)
C(111)	1040(40)	440(30)	480(30)	50(20)	400(30)	80(30)
C(112)	550(30)	750(30)	520(30)	-170(20)	270(20)	-120(20)
C(113)	370(20)	990(40)	540(30)	90(30)	230(20)	90(20)
C(114)	490(20)	710(30)	700(30)	280(20)	380(20)	140(20)
C(115)	420(20)	930(40)	610(30)	210(30)	210(20)	-60(20)
C(116)	630(30)	860(40)	390(30)	150(20)	30(20)	160(30)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for MJA08 (CCDC 163590).

	x	y	z	U_{iso}
H(1A)	4297	1441	2977	22
H(1B)	3959	1133	2354	22
H(2A)	3231	2578	1698	24
H(2B)	3447	3725	1779	24
H(3A)	4096	4284	2814	20
H(3B)	4653	3614	3162	20
H(4A)	800	1542	3682	24
H(4B)	1234	1457	4311	24
H(5A)	875	4363	3533	24
H(5B)	415	3486	3246	24
H(6A)	1832	3089	4830	25
H(6B)	1594	4195	4608	25
H(8)	4375	4272	1990	31
H(9)	5106	4406	1754	38
H(10)	5714	3029	1871	36
H(11)	5571	1516	2229	28
H(12)	4833	1385	2458	27
H(14)	4336	425	3588	28
H(15)	4502	-981	4141	29
H(16)	3738	-2001	4051	29
H(17)	2806	-1642	3379	30
H(18)	2639	-249	2821	26
H(20)	3355	26	1883	30
H(21)	2679	-829	1126	38
H(22)	1706	-673	872	44
H(23)	1403	383	1356	39
H(24)	2080	1283	2103	30
H(26)	2366	2448	1126	31
H(27)	1442	2251	420	37
H(28)	660	2975	472	42
H(29)	815	3912	1228	43
H(30)	1730	4089	1946	33
H(32)	2484	5060	1403	41
H(33)	2462	6821	1416	50
H(34)	2853	7700	2235	42
H(35)	3259	6804	3041	32
H(36)	3248	5038	3036	24
H(38)	4513	5321	3521	29
H(39)	4772	6689	4115	36
H(40)	4606	6644	4863	35
H(41)	4170	5231	5009	33
H(42)	3883	3877	4399	28
H(44)	4005	2075	4297	22
H(45)	4683	1041	4963	25
H(46)	5572	743	4992	29
H(47)	5782	1500	4355	28
H(48)	5117	2564	3697	24
H(50)	310	1728	4214	35

H(51)	-455	2023	4395	47
H(52)	-652	3668	4561	57
H(53)	-95	5012	4529	55
H(54)	682	4702	4361	43
H(56)	2641	30	4044	26
H(57)	3396	-648	4812	34
H(58)	3558	-133	5667	39
H(59)	2909	956	5753	37
H(60)	2128	1588	4988	29
H(62)	1140	-317	3820	31
H(63)	760	-1710	3257	37
H(64)	870	-1875	2481	39
H(65)	1382	-658	2278	40
H(66)	1761	751	2841	29
H(68)	1192	2467	2134	29
H(69)	631	1348	1448	35
H(70)	-155	544	1459	43
H(71)	-389	909	2147	37
H(72)	143	2075	2809	28
H(74)	291	3961	1995	27
H(75)	98	5410	1464	33
H(76)	757	6749	1743	33
H(77)	1579	6662	2578	29
H(78)	1751	5256	3131	23
H(80)	3017	4973	4161	27
H(81)	3067	6675	3974	34
H(82)	2338	7786	3879	36
H(83)	1565	7187	3991	34
H(84)	1525	5493	4197	27
H(86)	3288	2643	4543	26
H(87)	4136	2258	5324	30
H(88)	4267	2813	6160	35
H(89)	3543	3722	6223	39
H(90)	2703	4145	5444	35
H(101)	3715	7090	1714	46
H(102)	3024	6746	842	58
H(103)	2905	7803	143	67
H(104)	3481	9220	307	74
H(105)	4168	9616	1195	57
H(106)	4290	8531	1899	43
H(111)	8831	5239	-145	76
H(112)	9748	4674	464	72
H(113)	9865	3058	817	75
H(114)	9098	1965	529	71
H(115)	8182	2509	-92	80
H(116)	8048	4154	-415	85

4: $[PhB(CH_2PPh_2)(CH_2P(O)Ph_2)_2]CoI$

Table 1. Crystal data and structure refinement for dmj02.

Identification code	dmj02	
Empirical formula	C57 H53 B Co I O2 P3	
Formula weight	1059.54	
Temperature	98(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.916(3) Å	α= 90°.
	b = 18.582(4) Å	β= 106.262(3)°.
	c = 21.674(5) Å	γ = 90°.
Volume	4993.7(18) $Å^3$	
Z	4	
Density (calculated)	1.409 g/cm^3	
Absorption coefficient	1.100 mm^{-1}	
F(000)	2164	
Crystal size	0.22 x 0.089 x 0.16 mm^3	
Crystal Color	Electric Blue	
Theta range for data collection	1.47 to 23.32°.	
Index ranges	-14<=h<=14, -20<=k<=20, -24<=l<=24	
Reflections collected	54319	
Independent reflections	7213 [R(int) = 0.0773]	
Completeness to theta = 23.32°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7213 / 0 / 586	
Goodness-of-fit on F^2	1.755	
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0602	
R indices (all data)	R1 = 0.0547, wR2 = 0.0637	
Largest diff. peak and hole	1.060 and -1.086 $e.Å^{-3}$	
CCDC Depository Number	169215	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for dmj02. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	10164(1)	7135(1)	695(1)	15(1)
I	11290(1)	7597(1)	-28(1)	22(1)
O(1)	8874(2)	6591(1)	287(1)	18(1)
O(2)	10919(2)	6520(1)	1399(1)	17(1)
P(3)	9622(1)	8038(1)	1287(1)	16(1)
P(4)	10692(1)	6156(1)	1972(1)	16(1)
P(5)	7873(1)	6355(1)	464(1)	16(1)
B	8521(3)	6874(2)	1866(2)	15(1)
C(1)	7730(3)	6927(2)	2335(2)	14(1)
C(2)	8076(3)	6883(2)	3007(2)	18(1)
C(3)	7375(3)	6945(2)	3383(2)	23(1)
C(4)	6293(3)	7066(2)	3107(2)	23(1)
C(5)	5924(3)	7132(2)	2453(2)	23(1)
C(6)	6634(3)	7064(2)	2081(2)	20(1)
C(7)	9729(3)	6582(2)	2298(2)	15(1)
C(8)	8545(3)	7717(2)	1598(2)	17(1)
C(9)	7960(3)	6271(2)	1292(2)	16(1)
C(10)	10232(3)	5249(2)	1752(2)	13(1)
C(11)	10022(3)	4780(2)	2201(2)	18(1)
C(12)	9609(3)	4106(2)	2011(2)	19(1)
C(13)	9406(3)	3891(2)	1378(2)	22(1)
C(14)	9620(3)	4353(2)	931(2)	20(1)
C(15)	10039(3)	5030(2)	1119(2)	17(1)
C(16)	11953(3)	6087(2)	2597(2)	17(1)
C(17)	12353(3)	6687(2)	2963(2)	24(1)
C(18)	13349(3)	6668(2)	3421(2)	26(1)
C(19)	13946(3)	6048(2)	3511(2)	26(1)
C(20)	13556(3)	5448(2)	3149(2)	32(1)
C(21)	12568(3)	5463(2)	2695(2)	25(1)
C(22)	6800(3)	6981(2)	119(2)	20(1)
C(23)	6994(3)	7546(2)	-257(2)	32(1)

C(24)	6187(4)	8047(2)	-514(2)	44(1)
C(25)	5205(4)	7984(2)	-394(2)	41(1)
C(26)	4995(3)	7420(2)	-37(2)	34(1)
C(27)	5783(3)	6919(2)	216(2)	24(1)
C(28)	7472(3)	5501(2)	75(2)	15(1)
C(29)	7760(3)	5341(2)	-476(2)	18(1)
C(30)	7494(3)	4687(2)	-781(2)	23(1)
C(31)	6933(3)	4183(2)	-536(2)	23(1)
C(32)	6638(3)	4337(2)	15(2)	25(1)
C(33)	6901(3)	4994(2)	320(2)	21(1)
C(34)	10775(3)	8261(2)	1968(2)	16(1)
C(35)	10694(3)	8423(2)	2580(2)	19(1)
C(36)	11600(3)	8600(2)	3072(2)	21(1)
C(37)	12599(3)	8602(2)	2964(2)	22(1)
C(38)	12693(3)	8444(2)	2358(2)	24(1)
C(39)	11793(3)	8270(2)	1869(2)	21(1)
C(40)	9178(3)	8917(2)	939(2)	17(1)
C(41)	8907(3)	9451(2)	1313(2)	21(1)
C(42)	8549(3)	10115(2)	1049(2)	25(1)
C(43)	8456(3)	10248(2)	413(2)	25(1)
C(44)	8713(3)	9724(2)	37(2)	29(1)
C(45)	9086(3)	9057(2)	300(2)	25(1)
C(46)	6503(3)	5123(2)	2185(2)	26(1)
C(47)	5551(3)	5105(2)	1692(2)	27(1)
C(48)	5266(3)	4498(2)	1317(2)	27(1)
C(49)	5932(3)	3899(2)	1440(2)	26(1)
C(50)	6877(3)	3915(2)	1927(2)	27(1)
C(51)	7168(3)	4527(2)	2297(2)	26(1)
C(52)	5462(5)	8803(3)	1156(2)	57(1)
C(53)	5831(5)	9425(4)	1015(3)	103(3)
C(55)	4084(5)	9912(4)	871(5)	191(6)
C(56)	3724(4)	9275(3)	1001(2)	60(2)
C(57)	4411(5)	8723(3)	1147(2)	53(1)
C(54)	5147(6)	9985(4)	861(5)	241(8)

Table 3. Bond lengths [Å] and angles [°] for dmj02.

Co-O(1)	1.937(2)
Co-O(2)	1.937(2)
Co-P(3)	2.3347(11)
Co-I	2.5660(6)
O(1)-P(5)	1.513(2)
O(2)-P(4)	1.514(2)
P(3)-C(8)	1.808(3)
P(3)-C(40)	1.823(4)
P(3)-C(34)	1.826(4)
P(4)-C(7)	1.778(3)
P(4)-C(10)	1.807(3)
P(4)-C(16)	1.807(4)
P(5)-C(9)	1.773(3)
P(5)-C(22)	1.803(4)
P(5)-C(28)	1.803(4)
B-C(1)	1.633(5)
B-C(7)	1.670(5)
B-C(8)	1.674(5)
B-C(9)	1.681(5)
C(1)-C(6)	1.392(5)
C(1)-C(2)	1.402(5)
C(2)-C(3)	1.381(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.376(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.369(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(5)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900

C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(15)	1.386(5)
C(10)-C(11)	1.389(5)
C(11)-C(12)	1.378(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.381(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.379(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.384(5)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(5)
C(16)-C(21)	1.388(5)
C(17)-C(18)	1.388(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.370(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.376(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.375(5)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(27)	1.391(5)
C(22)-C(23)	1.394(5)
C(23)-C(24)	1.393(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.371(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.373(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.376(5)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.379(5)

C(28)-C(33)	1.390(5)
C(29)-C(30)	1.381(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.380(5)
C(30)-H(30)	0.9500
C(31)-C(32)	1.381(5)
C(31)-H(31)	0.9500
C(32)-C(33)	1.383(5)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.391(5)
C(34)-C(35)	1.392(5)
C(35)-C(36)	1.385(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.375(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.384(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.374(5)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.381(5)
C(40)-C(41)	1.386(5)
C(41)-C(42)	1.384(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.373(5)
C(42)-H(42)	0.9500
C(43)-C(44)	1.368(5)
C(43)-H(43)	0.9500
C(44)-C(45)	1.393(5)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.379(5)
C(46)-C(47)	1.385(5)
C(46)-H(46)	0.9500
C(47)-C(48)	1.380(5)

C(47)-H(47)	0.9500
C(48)-C(49)	1.387(5)
C(48)-H(48)	0.9500
C(49)-C(50)	1.372(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.383(5)
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(52)-C(53)	1.317(7)
C(52)-C(57)	1.360(6)
C(52)-H(52)	0.9500
C(53)-C(54)	1.346(10)
C(53)-H(53)	0.9500
C(55)-C(56)	1.332(7)
C(55)-C(54)	1.385(11)
C(55)-H(55)	0.9500
C(56)-C(57)	1.335(6)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(54)-H(54)	0.9500

O(1)-Co-O(2)	103.32(10)
O(1)-Co-P(3)	105.90(7)
O(2)-Co-P(3)	98.85(7)
O(1)-Co-I	117.25(7)
O(2)-Co-I	115.55(7)
P(3)-Co-I	113.83(3)
P(5)-O(1)-Co	136.27(15)
P(4)-O(2)-Co	137.65(14)
C(8)-P(3)-C(40)	105.27(16)
C(8)-P(3)-C(34)	108.15(17)
C(40)-P(3)-C(34)	102.83(16)
C(8)-P(3)-Co	110.41(11)
C(40)-P(3)-Co	121.60(13)
C(34)-P(3)-Co	107.78(12)
O(2)-P(4)-C(7)	116.44(15)

O(2)-P(4)-C(10)	108.92(15)
C(7)-P(4)-C(10)	107.79(16)
O(2)-P(4)-C(16)	107.82(15)
C(7)-P(4)-C(16)	108.54(16)
C(10)-P(4)-C(16)	106.95(16)
O(1)-P(5)-C(9)	117.73(15)
O(1)-P(5)-C(22)	108.65(16)
C(9)-P(5)-C(22)	107.49(17)
O(1)-P(5)-C(28)	106.92(15)
C(9)-P(5)-C(28)	108.88(16)
C(22)-P(5)-C(28)	106.65(16)
C(1)-B-C(7)	108.7(3)
C(1)-B-C(8)	103.6(3)
C(7)-B-C(8)	113.2(3)
C(1)-B-C(9)	106.6(3)
C(7)-B-C(9)	109.9(3)
C(8)-B-C(9)	114.4(3)
C(6)-C(1)-C(2)	114.5(3)
C(6)-C(1)-B	120.6(3)
C(2)-C(1)-B	124.8(3)
C(3)-C(2)-C(1)	122.5(3)
C(3)-C(2)-H(2)	118.8
C(1)-C(2)-H(2)	118.8
C(4)-C(3)-C(2)	120.8(4)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	118.8(3)
C(5)-C(4)-H(4)	120.6
C(3)-C(4)-H(4)	120.6
C(4)-C(5)-C(6)	119.9(3)
C(4)-C(5)-H(5)	120.0
C(6)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	123.6(4)
C(5)-C(6)-H(6)	118.2
C(1)-C(6)-H(6)	118.2
B-C(7)-P(4)	124.8(2)

B-C(7)-H(7A)	106.1
P(4)-C(7)-H(7A)	106.1
B-C(7)-H(7B)	106.1
P(4)-C(7)-H(7B)	106.1
H(7A)-C(7)-H(7B)	106.3
B-C(8)-P(3)	121.9(2)
B-C(8)-H(8A)	106.9
P(3)-C(8)-H(8A)	106.9
B-C(8)-H(8B)	106.9
P(3)-C(8)-H(8B)	106.9
H(8A)-C(8)-H(8B)	106.7
B-C(9)-P(5)	125.6(2)
B-C(9)-H(9A)	105.9
P(5)-C(9)-H(9A)	105.9
B-C(9)-H(9B)	105.9
P(5)-C(9)-H(9B)	105.9
H(9A)-C(9)-H(9B)	106.2
C(15)-C(10)-C(11)	119.6(3)
C(15)-C(10)-P(4)	119.4(3)
C(11)-C(10)-P(4)	121.0(3)
C(12)-C(11)-C(10)	119.7(4)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	120.6(3)
C(11)-C(12)-H(12)	119.7
C(13)-C(12)-H(12)	119.7
C(14)-C(13)-C(12)	119.8(3)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(13)-C(14)-C(15)	119.9(4)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(10)	120.3(3)
C(14)-C(15)-H(15)	119.9
C(10)-C(15)-H(15)	119.9
C(17)-C(16)-C(21)	118.7(3)

C(17)-C(16)-P(4)	119.1(3)
C(21)-C(16)-P(4)	122.1(3)
C(16)-C(17)-C(18)	120.8(3)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(19)-C(18)-C(17)	119.7(4)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(20)	120.0(4)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
C(21)-C(20)-C(19)	120.6(4)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(16)	120.2(4)
C(20)-C(21)-H(21)	119.9
C(16)-C(21)-H(21)	119.9
C(27)-C(22)-C(23)	118.8(3)
C(27)-C(22)-P(5)	122.2(3)
C(23)-C(22)-P(5)	119.0(3)
C(24)-C(23)-C(22)	120.1(4)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(25)-C(24)-C(23)	119.7(4)
C(25)-C(24)-H(24)	120.2
C(23)-C(24)-H(24)	120.2
C(24)-C(25)-C(26)	120.7(4)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(25)-C(26)-C(27)	120.1(4)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(26)-C(27)-C(22)	120.6(4)
C(26)-C(27)-H(27)	119.7
C(22)-C(27)-H(27)	119.7
C(29)-C(28)-C(33)	119.0(3)

C(29)-C(28)-P(5)	118.8(3)
C(33)-C(28)-P(5)	122.2(3)
C(28)-C(29)-C(30)	120.9(3)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(31)-C(30)-C(29)	120.0(4)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	119.6(4)
C(30)-C(31)-H(31)	120.2
C(32)-C(31)-H(31)	120.2
C(31)-C(32)-C(33)	120.4(4)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(32)-C(33)-C(28)	120.1(3)
C(32)-C(33)-H(33)	120.0
C(28)-C(33)-H(33)	120.0
C(39)-C(34)-C(35)	118.1(3)
C(39)-C(34)-P(3)	118.1(3)
C(35)-C(34)-P(3)	123.9(3)
C(36)-C(35)-C(34)	120.9(3)
C(36)-C(35)-H(35)	119.6
C(34)-C(35)-H(35)	119.6
C(37)-C(36)-C(35)	120.0(4)
C(37)-C(36)-H(36)	120.0
C(35)-C(36)-H(36)	120.0
C(36)-C(37)-C(38)	119.8(4)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(39)-C(38)-C(37)	120.1(4)
C(39)-C(38)-H(38)	120.0
C(37)-C(38)-H(38)	120.0
C(38)-C(39)-C(34)	121.1(4)
C(38)-C(39)-H(39)	119.4
C(34)-C(39)-H(39)	119.4
C(45)-C(40)-C(41)	119.0(3)

C(45)-C(40)-P(3)	120.9(3)
C(41)-C(40)-P(3)	120.1(3)
C(42)-C(41)-C(40)	120.5(4)
C(42)-C(41)-H(41)	119.8
C(40)-C(41)-H(41)	119.8
C(43)-C(42)-C(41)	120.0(4)
C(43)-C(42)-H(42)	120.0
C(41)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	120.2(4)
C(44)-C(43)-H(43)	119.9
C(42)-C(43)-H(43)	119.9
C(43)-C(44)-C(45)	120.1(4)
C(43)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(40)-C(45)-C(44)	120.2(4)
C(40)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(51)-C(46)-C(47)	119.4(4)
C(51)-C(46)-H(46)	120.3
C(47)-C(46)-H(46)	120.3
C(48)-C(47)-C(46)	120.5(4)
C(48)-C(47)-H(47)	119.8
C(46)-C(47)-H(47)	119.8
C(47)-C(48)-C(49)	119.6(4)
C(47)-C(48)-H(48)	120.2
C(49)-C(48)-H(48)	120.2
C(50)-C(49)-C(48)	120.1(4)
C(50)-C(49)-H(49)	120.0
C(48)-C(49)-H(49)	120.0
C(49)-C(50)-C(51)	120.2(4)
C(49)-C(50)-H(50)	119.9
C(51)-C(50)-H(50)	119.9
C(46)-C(51)-C(50)	120.2(4)
C(46)-C(51)-H(51)	119.9
C(50)-C(51)-H(51)	119.9
C(53)-C(52)-C(57)	121.2(6)

C(53)-C(52)-H(52)	119.4
C(57)-C(52)-H(52)	119.4
C(52)-C(53)-C(54)	118.7(6)
C(52)-C(53)-H(53)	120.6
C(54)-C(53)-H(53)	120.6
C(56)-C(55)-C(54)	119.8(6)
C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1
C(55)-C(56)-C(57)	119.0(6)
C(55)-C(56)-H(56)	120.5
C(57)-C(56)-H(56)	120.5
C(56)-C(57)-C(52)	120.9(5)
C(56)-C(57)-H(57)	119.6
C(52)-C(57)-H(57)	119.6
C(53)-C(54)-C(55)	120.3(6)
C(53)-C(54)-H(54)	119.8
C(55)-C(54)-H(54)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for dmj02. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co	18(1)	12(1)	15(1)	0(1)	4(1)	-2(1)
I	30(1)	18(1)	22(1)	0(1)	13(1)	-3(1)
O(1)	20(2)	18(1)	17(2)	-2(1)	5(1)	-4(1)
O(2)	21(1)	13(1)	19(2)	1(1)	7(1)	0(1)
P(3)	17(1)	14(1)	16(1)	0(1)	5(1)	-1(1)
P(4)	17(1)	13(1)	16(1)	0(1)	4(1)	1(1)
P(5)	18(1)	15(1)	15(1)	-1(1)	4(1)	-2(1)
B	16(2)	14(2)	14(3)	-3(2)	3(2)	-3(2)
C(1)	16(2)	5(2)	20(2)	-2(2)	6(2)	-4(2)
C(2)	16(2)	16(2)	22(2)	1(2)	6(2)	1(2)
C(3)	32(3)	22(2)	15(2)	-1(2)	9(2)	-1(2)
C(4)	33(3)	15(2)	29(3)	-5(2)	20(2)	-3(2)
C(5)	16(2)	21(2)	33(3)	-6(2)	10(2)	0(2)
C(6)	24(2)	18(2)	17(2)	-2(2)	4(2)	0(2)
C(7)	20(2)	12(2)	15(2)	0(2)	7(2)	-4(2)
C(8)	14(2)	18(2)	17(2)	-4(2)	4(2)	1(2)
C(9)	12(2)	16(2)	19(2)	1(2)	5(2)	-1(2)
C(10)	12(2)	13(2)	15(2)	0(2)	4(2)	2(2)
C(11)	14(2)	19(2)	23(2)	-1(2)	5(2)	2(2)
C(12)	17(2)	15(2)	26(3)	6(2)	7(2)	0(2)
C(13)	13(2)	15(2)	34(3)	-3(2)	3(2)	-1(2)
C(14)	23(2)	18(2)	19(2)	-4(2)	3(2)	6(2)
C(15)	14(2)	12(2)	24(2)	5(2)	4(2)	3(2)
C(16)	18(2)	18(2)	15(2)	2(2)	8(2)	-3(2)
C(17)	20(2)	19(2)	28(3)	0(2)	0(2)	5(2)
C(18)	21(2)	26(2)	26(3)	-9(2)	1(2)	-2(2)
C(19)	17(2)	34(3)	23(3)	5(2)	-2(2)	1(2)
C(20)	23(2)	21(2)	45(3)	2(2)	0(2)	10(2)
C(21)	25(2)	19(2)	30(3)	-3(2)	5(2)	4(2)
C(22)	26(2)	16(2)	14(2)	-4(2)	-3(2)	1(2)
C(23)	38(3)	26(3)	26(2)	1(2)	3(2)	-1(2)

C(24)	57(3)	21(3)	47(3)	14(2)	3(3)	10(2)
C(25)	42(3)	27(3)	39(3)	-7(2)	-13(2)	13(2)
C(26)	23(2)	31(3)	40(3)	-16(2)	-3(2)	7(2)
C(27)	22(2)	20(2)	25(2)	-7(2)	0(2)	0(2)
C(28)	12(2)	15(2)	14(2)	2(2)	0(2)	3(2)
C(29)	16(2)	17(2)	18(2)	1(2)	2(2)	3(2)
C(30)	20(2)	29(3)	19(2)	-4(2)	6(2)	3(2)
C(31)	23(2)	17(2)	26(3)	-5(2)	0(2)	1(2)
C(32)	31(3)	18(2)	25(3)	0(2)	7(2)	-9(2)
C(33)	24(2)	23(2)	16(2)	-3(2)	8(2)	-5(2)
C(34)	17(2)	11(2)	21(2)	0(2)	7(2)	-4(2)
C(35)	17(2)	18(2)	22(2)	-2(2)	6(2)	-1(2)
C(36)	24(2)	18(2)	19(2)	-7(2)	6(2)	2(2)
C(37)	23(2)	16(2)	23(3)	-6(2)	1(2)	-1(2)
C(38)	17(2)	27(2)	33(3)	-8(2)	12(2)	-7(2)
C(39)	25(2)	20(2)	20(2)	-3(2)	8(2)	-3(2)
C(40)	15(2)	15(2)	21(2)	0(2)	5(2)	-5(2)
C(41)	24(2)	17(2)	25(2)	-1(2)	11(2)	-2(2)
C(42)	22(2)	14(2)	38(3)	-5(2)	9(2)	-3(2)
C(43)	24(2)	14(2)	33(3)	7(2)	2(2)	3(2)
C(44)	39(3)	25(2)	21(2)	7(2)	7(2)	6(2)
C(45)	27(2)	20(2)	26(3)	-1(2)	7(2)	4(2)
C(46)	33(3)	24(3)	22(3)	-1(2)	13(2)	-9(2)
C(47)	30(3)	27(3)	29(3)	9(2)	15(2)	2(2)
C(48)	20(2)	38(3)	23(3)	6(2)	6(2)	-7(2)
C(49)	33(3)	26(3)	22(3)	-3(2)	14(2)	-14(2)
C(50)	28(3)	25(2)	32(3)	7(2)	15(2)	2(2)
C(51)	18(2)	35(3)	23(3)	6(2)	3(2)	1(2)
C(52)	71(4)	56(4)	46(4)	-13(3)	19(3)	3(3)
C(53)	65(4)	118(6)	91(5)	58(4)	-36(4)	-59(4)
C(55)	84(6)	58(5)	327(13)	92(6)	-112(7)	-32(4)
C(56)	55(4)	57(4)	54(4)	12(3)	-9(3)	4(3)
C(57)	83(4)	32(3)	52(4)	-1(3)	33(3)	-3(3)
C(54)	93(6)	113(7)	393(16)	185(9)	-134(8)	-68(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for dmj02.

	x	y	z	U(eq)
H(2)	8820	6807	3212	21
H(3)	7644	6904	3837	27
H(4)	5811	7103	3366	28
H(5)	5181	7223	2254	27
H(6)	6358	7115	1629	24
H(7A)	9592	6243	2619	18
H(7B)	10099	7004	2542	18
H(8A)	8519	8042	1956	20
H(8B)	7863	7790	1255	20
H(9A)	7211	6203	1314	19
H(9B)	8338	5811	1433	19
H(11)	10162	4923	2638	22
H(12)	9462	3786	2318	23
H(13)	9120	3426	1251	26
H(14)	9480	4207	496	24
H(15)	10195	5345	812	21
H(17)	11941	7118	2900	29
H(18)	13616	7084	3670	31
H(19)	14628	6032	3823	31
H(20)	13972	5019	3212	38
H(21)	12306	5045	2448	30
H(23)	7678	7590	-337	38
H(24)	6317	8431	-772	53
H(25)	4662	8335	-558	49
H(26)	4306	7376	35	41
H(27)	5632	6527	459	28
H(29)	8147	5686	-647	21
H(30)	7697	4585	-1161	27
H(31)	6751	3732	-744	28
H(32)	6253	3991	185	30

H(33)	6692	5098	697	25
H(35)	10008	8412	2660	23
H(36)	11530	8720	3485	25
H(37)	13223	8711	3305	26
H(38)	13381	8456	2280	29
H(39)	11868	8153	1457	25
H(41)	8968	9360	1753	25
H(42)	8368	10479	1309	29
H(43)	8213	10704	233	30
H(44)	8637	9816	-405	34
H(45)	9278	8698	40	29
H(46)	6698	5542	2443	31
H(47)	5091	5514	1613	33
H(48)	4617	4491	975	33
H(49)	5733	3476	1188	31
H(50)	7333	3504	2009	32
H(51)	7827	4538	2630	31
H(52)	5938	8405	1266	69
H(53)	6565	9476	1021	124
H(55)	3614	10316	786	229
H(56)	2988	9213	990	72
H(57)	4163	8268	1246	64
H(54)	5394	10433	745	289

5: [PhBP$_3$]Co(O-2,6-dimethylphenyl)

Table 1. Crystal data and structure refinement for BP3CoOAr.

Identification code	dmj11	
Empirical formula	C53 H50 B Co O P3	
Formula weight	865.58	
Temperature	96(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 17.2447(14) Å	α= 90°.
	b = 16.4840(13) Å	β= 109.1810(10)°.
	c = 16.4939(13) Å	γ = 90°.
Volume	4428.3(6) Å^3	
Z	4	
Density (calculated)	1.298 Mg/m^3	
Absorption coefficient	0.535 mm^{-1}	
F(000)	1812	
Crystal size	0.170 x 0.185 x 0.192 mm^3	
Theta range for data collection	1.76 to 28.61°.	
Index ranges	-23<=h<=22, -21<=k<=21, -21<=l<=22	
Reflections collected	45708	
Independent reflections	10456 [R(int) = 0.0561]	
Completeness to theta = 28.61°	94.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10456 / 2 / 534	
Goodness-of-fit on F^2	1.661	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0612	
R indices (all data)	R1 = 0.0454, wR2 = 0.0624	
Absolute structure parameter	-0.004(8)	
Largest diff. peak and hole	1.133 and -0.475 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for BP3CoOAr. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	6900(1)	7508(1)	607(1)	18(1)
P(1)	7507(1)	8795(1)	761(1)	18(1)
P(2)	7121(1)	7230(1)	-707(1)	19(1)
P(3)	8089(1)	6909(1)	1529(1)	17(1)
O	5983(1)	7632(1)	944(1)	23(1)
B	8783(2)	7836(2)	359(2)	18(1)
C(1)	9656(1)	8003(1)	218(1)	20(1)
C(2)	10420(1)	7780(1)	792(2)	24(1)
C(3)	11155(2)	7980(2)	672(2)	28(1)
C(4)	11159(2)	8411(2)	-35(2)	29(1)
C(5)	10415(2)	8633(2)	-641(2)	30(1)
C(6)	9687(2)	8429(1)	-511(2)	27(1)
C(7)	8313(1)	8745(1)	284(1)	19(1)
C(8)	8238(1)	7221(1)	-428(1)	20(1)
C(9)	8947(1)	7400(1)	1314(1)	20(1)
C(10)	6828(1)	9656(1)	325(1)	19(1)
C(11)	5993(2)	9588(2)	195(2)	25(1)

C(12)	5471(2)	10240(2)	-121(2)	31(1)
C(13)	5781(2)	10963(2)	-304(2)	34(1)
C(14)	6612(2)	11037(2)	-171(2)	33(1)
C(15)	7131(2)	10389(1)	137(2)	27(1)
C(16)	7983(1)	9112(1)	1882(1)	18(1)
C(17)	7474(2)	9171(1)	2374(2)	26(1)
C(18)	7775(2)	9416(2)	3219(2)	32(1)
C(19)	8600(2)	9602(1)	3577(2)	30(1)
C(20)	9111(2)	9538(1)	3102(2)	30(1)
C(21)	8797(2)	9296(1)	2244(2)	26(1)
C(22)	6752(1)	6300(1)	-1318(1)	20(1)
C(23)	6191(2)	6302(2)	-2141(2)	26(1)
C(24)	5944(2)	5581(2)	-2581(2)	29(1)
C(25)	6244(2)	4850(2)	-2207(2)	27(1)
C(26)	6801(2)	4841(1)	-1390(2)	27(1)
C(27)	7053(2)	5559(1)	-945(2)	26(1)
C(28)	6735(1)	8030(1)	-1507(1)	21(1)
C(29)	6060(2)	8476(1)	-1493(2)	25(1)
C(30)	5729(2)	9073(2)	-2100(2)	33(1)
C(31)	6075(2)	9226(2)	-2728(2)	34(1)
C(32)	6739(2)	8789(2)	-2756(2)	33(1)
C(33)	7079(2)	8189(1)	-2153(2)	26(1)
C(34)	8202(1)	7057(1)	2659(1)	20(1)
C(35)	8975(2)	7100(2)	3285(2)	29(1)
C(36)	9057(2)	7222(2)	4139(2)	34(1)
C(37)	8366(2)	7308(1)	4380(2)	31(1)
C(38)	7597(2)	7262(1)	3767(2)	29(1)
C(39)	7518(2)	7139(1)	2903(2)	23(1)
C(40)	8232(1)	5810(1)	1465(1)	20(1)
C(41)	8766(1)	5461(1)	1090(1)	23(1)
C(42)	8800(2)	4622(2)	1019(2)	29(1)
C(43)	8320(2)	4128(2)	1324(2)	32(1)
C(44)	7799(2)	4470(2)	1707(2)	36(1)
C(45)	7745(2)	5300(1)	1767(2)	28(1)
C(46)	5452(1)	7163(1)	1175(1)	21(1)
C(47)	5219(1)	6391(1)	807(2)	23(1)
C(48)	4623(2)	5962(2)	1030(2)	29(1)
C(49)	4272(2)	6268(2)	1607(2)	31(1)
C(50)	4525(2)	7004(2)	1984(2)	29(1)
C(51)	5117(1)	7468(1)	1785(1)	23(1)
C(52)	5409(2)	8263(2)	2224(2)	31(1)
C(53)	5610(2)	6050(2)	189(2)	29(1)

Table 3. Bond lengths [Å] and angles [°] for BP3CoOAr.

Co-O	1.8513(15)
Co-B	3.4463(26)
Co-P(3)	2.3318(7)
Co-P(1)	2.3430(6)
Co-P(2)	2.3656(7)
P(1)-C(7)	1.809(2)
P(1)-C(10)	1.830(2)
P(1)-C(16)	1.835(2)
P(2)-C(8)	1.829(2)
P(2)-C(28)	1.829(2)
P(2)-C(22)	1.830(2)

P(3)-C(9)	1.821(2)
P(3)-C(34)	1.827(2)
P(3)-C(40)	1.836(2)
O-C(46)	1.346(3)
B-C(1)	1.621(3)
B-C(9)	1.669(3)
B-C(8)	1.671(3)
B-C(7)	1.689(3)
C(1)-C(2)	1.395(3)
C(1)-C(6)	1.408(3)
C(2)-C(3)	1.384(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.367(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.391(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.383(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.390(3)
C(10)-C(15)	1.390(3)
C(11)-C(12)	1.388(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.382(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.381(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.378(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(21)	1.366(3)
C(16)-C(17)	1.382(3)
C(17)-C(18)	1.379(3)
C(17)-H(17)	0.9500
C(18)-C(19)	1.383(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.363(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.397(3)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.385(3)
C(22)-C(27)	1.389(3)
C(23)-C(24)	1.384(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.375(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.374(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(3)

C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.383(3)
C(28)-C(33)	1.404(3)
C(29)-C(30)	1.386(3)
C(29)-H(29)	0.9500
C(30)-C(31)	1.377(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.367(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.388(3)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.371(3)
C(34)-C(35)	1.394(3)
C(35)-C(36)	1.385(3)
C(35)-H(35)	0.9500
C(36)-C(37)	1.380(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.381(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.400(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(40)-C(45)	1.391(3)
C(40)-C(41)	1.392(3)
C(41)-C(42)	1.391(3)
C(41)-H(41)	0.9500
C(42)-C(43)	1.368(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.378(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.378(3)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(46)-C(51)	1.408(3)
C(46)-C(47)	1.411(3)
C(47)-C(48)	1.392(3)
C(47)-C(53)	1.505(3)
C(48)-C(49)	1.380(3)
C(48)-H(48)	0.9500
C(49)-C(50)	1.368(3)
C(49)-H(49)	0.9500
C(50)-C(51)	1.398(3)
C(50)-H(50)	0.9500
C(51)-C(52)	1.503(3)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800

O-Co-P(3)	120.39(5)
O-Co-P(1)	105.27(5)
P(3)-Co-P(1)	92.72(2)

O-Co-P(2)	134.93(5)
P(3)-Co-P(2)	98.27(2)
P(1)-Co-P(2)	94.22(2)
C(7)-P(1)-C(10)	110.43(10)
C(7)-P(1)-C(16)	107.31(11)
C(10)-P(1)-C(16)	101.06(9)
C(7)-P(1)-Co	106.94(8)
C(10)-P(1)-Co	117.02(8)
C(16)-P(1)-Co	113.72(7)
C(8)-P(2)-C(28)	106.92(10)
C(8)-P(2)-C(22)	106.15(10)
C(28)-P(2)-C(22)	103.20(10)
C(8)-P(2)-Co	104.14(7)
C(28)-P(2)-Co	113.07(8)
C(22)-P(2)-Co	122.39(7)
C(9)-P(3)-C(34)	108.54(10)
C(9)-P(3)-C(40)	107.11(11)
C(34)-P(3)-C(40)	102.65(10)
C(9)-P(3)-Co	106.34(7)
C(34)-P(3)-Co	112.64(8)
C(40)-P(3)-Co	119.14(8)
C(46)-O-Co	138.52(14)
C(1)-B-C(9)	109.36(18)
C(1)-B-C(8)	107.71(17)
C(9)-B-C(8)	110.49(18)
C(1)-B-C(7)	106.51(18)
C(9)-B-C(7)	112.24(18)
C(8)-B-C(7)	110.37(18)
C(2)-C(1)-C(6)	114.7(2)
C(2)-C(1)-B	124.9(2)
C(6)-C(1)-B	120.3(2)
C(3)-C(2)-C(1)	123.0(2)
C(3)-C(2)-H(2)	118.5
C(1)-C(2)-H(2)	118.5
C(4)-C(3)-C(2)	120.4(2)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.2(2)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(6)-C(5)-C(4)	119.6(2)
C(6)-C(5)-H(5)	120.2
C(4)-C(5)-H(5)	120.2
C(5)-C(6)-C(1)	123.0(2)
C(5)-C(6)-H(6)	118.5
C(1)-C(6)-H(6)	118.5
B-C(7)-P(1)	115.32(15)
B-C(7)-H(7A)	108.4
P(1)-C(7)-H(7A)	108.4
B-C(7)-H(7B)	108.4
P(1)-C(7)-H(7B)	108.4
H(7A)-C(7)-H(7B)	107.5
B-C(8)-P(2)	117.89(15)
B-C(8)-H(8A)	107.8
P(2)-C(8)-H(8A)	107.8
B-C(8)-H(8B)	107.8

P(2)-C(8)-H(8B)	107.8
H(8A)-C(8)-H(8B)	107.2
B-C(9)-P(3)	118.59(15)
B-C(9)-H(9A)	107.7
P(3)-C(9)-H(9A)	107.7
B-C(9)-H(9B)	107.7
P(3)-C(9)-H(9B)	107.7
H(9A)-C(9)-H(9B)	107.1
C(11)-C(10)-C(15)	118.8(2)
C(11)-C(10)-P(1)	119.67(17)
C(15)-C(10)-P(1)	121.50(18)
C(12)-C(11)-C(10)	120.5(2)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(13)-C(12)-C(11)	120.0(3)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	119.8(2)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(15)-C(14)-C(13)	120.3(2)
C(15)-C(14)-H(14)	119.8
C(13)-C(14)-H(14)	119.8
C(14)-C(15)-C(10)	120.6(2)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7
C(21)-C(16)-C(17)	119.1(2)
C(21)-C(16)-P(1)	124.01(18)
C(17)-C(16)-P(1)	116.84(18)
C(18)-C(17)-C(16)	120.8(2)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	119.4(2)
C(17)-C(18)-H(18)	120.3
C(19)-C(18)-H(18)	120.3
C(20)-C(19)-C(18)	120.4(2)
C(20)-C(19)-H(19)	119.8
C(18)-C(19)-H(19)	119.8
C(19)-C(20)-C(21)	119.7(2)
C(19)-C(20)-H(20)	120.2
C(21)-C(20)-H(20)	120.2
C(16)-C(21)-C(20)	120.5(2)
C(16)-C(21)-H(21)	119.7
C(20)-C(21)-H(21)	119.7
C(23)-C(22)-C(27)	118.3(2)
C(23)-C(22)-P(2)	122.87(18)
C(27)-C(22)-P(2)	118.81(18)
C(24)-C(23)-C(22)	120.6(2)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	120.7(2)
C(25)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(26)-C(25)-C(24)	119.2(2)
C(26)-C(25)-H(25)	120.4
C(24)-C(25)-H(25)	120.4

C(25)-C(26)-C(27)	120.5(2)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(26)-C(27)-C(22)	120.7(2)
C(26)-C(27)-H(27)	119.7
C(22)-C(27)-H(27)	119.7
C(29)-C(28)-C(33)	118.7(2)
C(29)-C(28)-P(2)	118.69(18)
C(33)-C(28)-P(2)	122.54(18)
C(28)-C(29)-C(30)	121.0(2)
C(28)-C(29)-H(29)	119.5
C(30)-C(29)-H(29)	119.5
C(31)-C(30)-C(29)	119.7(2)
C(31)-C(30)-H(30)	120.2
C(29)-C(30)-H(30)	120.2
C(32)-C(31)-C(30)	120.3(2)
C(32)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
C(31)-C(32)-C(33)	120.8(2)
C(31)-C(32)-H(32)	119.6
C(33)-C(32)-H(32)	119.6
C(32)-C(33)-C(28)	119.5(2)
C(32)-C(33)-H(33)	120.3
C(28)-C(33)-H(33)	120.3
C(39)-C(34)-C(35)	118.9(2)
C(39)-C(34)-P(3)	119.90(17)
C(35)-C(34)-P(3)	121.14(18)
C(36)-C(35)-C(34)	120.9(2)
C(36)-C(35)-H(35)	119.6
C(34)-C(35)-H(35)	119.6
C(37)-C(36)-C(35)	119.9(2)
C(37)-C(36)-H(36)	120.0
C(35)-C(36)-H(36)	120.0
C(36)-C(37)-C(38)	119.7(2)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.1(2)
C(37)-C(38)-H(38)	119.9
C(39)-C(38)-H(38)	119.9
C(34)-C(39)-C(38)	120.4(2)
C(34)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(45)-C(40)-C(41)	118.4(2)
C(45)-C(40)-P(3)	117.83(17)
C(41)-C(40)-P(3)	123.69(17)
C(42)-C(41)-C(40)	120.0(2)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(43)-C(42)-C(41)	120.8(2)
C(43)-C(42)-H(42)	119.6
C(41)-C(42)-H(42)	119.6
C(42)-C(43)-C(44)	119.4(2)
C(42)-C(43)-H(43)	120.3
C(44)-C(43)-H(43)	120.3
C(43)-C(44)-C(45)	120.6(2)
C(43)-C(44)-H(44)	119.7

C(45)-C(44)-H(44)	119.7
C(44)-C(45)-C(40)	120.8(2)
C(44)-C(45)-H(45)	119.6
C(40)-C(45)-H(45)	119.6
O-C(46)-C(51)	118.4(2)
O-C(46)-C(47)	121.4(2)
C(51)-C(46)-C(47)	120.2(2)
C(48)-C(47)-C(46)	118.4(2)
C(48)-C(47)-C(53)	121.6(2)
C(46)-C(47)-C(53)	120.0(2)
C(49)-C(48)-C(47)	121.6(2)
C(49)-C(48)-H(48)	119.2
C(47)-C(48)-H(48)	119.2
C(50)-C(49)-C(48)	119.5(2)
C(50)-C(49)-H(49)	120.3
C(48)-C(49)-H(49)	120.3
C(49)-C(50)-C(51)	121.7(2)
C(49)-C(50)-H(50)	119.1
C(51)-C(50)-H(50)	119.1
C(50)-C(51)-C(46)	118.4(2)
C(50)-C(51)-C(52)	121.3(2)
C(46)-C(51)-C(52)	120.3(2)
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(47)-C(53)-H(53A)	109.5
C(47)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(47)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for BP3CoOAr. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co	18(1)	19(1)	16(1)	0(1)	4(1)	-1(1)
P(1)	20(1)	18(1)	15(1)	-1(1)	5(1)	-1(1)
P(2)	20(1)	19(1)	16(1)	0(1)	5(1)	-1(1)
P(3)	18(1)	20(1)	14(1)	0(1)	4(1)	-1(1)
O	20(1)	23(1)	25(1)	3(1)	6(1)	-2(1)
B	20(1)	20(1)	13(1)	0(1)	5(1)	-1(1)
C(1)	24(1)	18(1)	18(1)	-5(1)	6(1)	-2(1)
C(2)	26(1)	25(1)	19(1)	0(1)	6(1)	-2(1)
C(3)	22(1)	34(2)	26(1)	2(1)	4(1)	1(1)
C(4)	24(1)	35(2)	32(2)	-4(1)	15(1)	-5(1)
C(5)	34(2)	35(2)	27(1)	5(1)	16(1)	0(1)
C(6)	25(1)	31(1)	25(1)	6(1)	8(1)	4(1)
C(7)	18(1)	23(1)	14(1)	0(1)	5(1)	-4(1)
C(8)	22(1)	21(1)	18(1)	0(1)	7(1)	2(1)

C(9)	18(1)	22(1)	19(1)	-1(1)	5(1)	-2(1)
C(10)	26(1)	21(1)	13(1)	1(1)	9(1)	3(1)
C(11)	27(1)	28(1)	21(1)	0(1)	9(1)	1(1)
C(12)	31(2)	40(2)	24(1)	1(1)	12(1)	7(1)
C(13)	45(2)	34(2)	25(1)	5(1)	14(1)	20(1)
C(14)	47(2)	27(1)	32(2)	9(1)	23(1)	6(1)
C(15)	33(2)	28(1)	22(1)	1(1)	13(1)	2(1)
C(16)	28(1)	13(1)	12(1)	-1(1)	6(1)	-2(1)
C(17)	30(2)	26(1)	21(1)	1(1)	9(1)	1(1)
C(18)	44(2)	38(2)	17(1)	-1(1)	15(1)	3(1)
C(19)	44(2)	25(1)	18(1)	-3(1)	8(1)	2(1)
C(20)	32(2)	30(1)	21(1)	-2(1)	1(1)	-6(1)
C(21)	32(2)	26(1)	20(1)	-1(1)	10(1)	-5(1)
C(22)	22(1)	20(1)	20(1)	-2(1)	11(1)	-3(1)
C(23)	23(1)	26(1)	26(1)	0(1)	6(1)	-3(1)
C(24)	22(1)	36(2)	27(1)	-7(1)	4(1)	-4(1)
C(25)	26(1)	29(1)	30(1)	-11(1)	16(1)	-9(1)
C(26)	38(2)	21(1)	28(1)	0(1)	18(1)	0(1)
C(27)	33(2)	26(1)	18(1)	-2(1)	8(1)	-5(1)
C(28)	26(1)	20(1)	14(1)	0(1)	0(1)	-6(1)
C(29)	24(1)	29(1)	20(1)	0(1)	3(1)	-1(1)
C(30)	31(2)	32(2)	30(2)	-1(1)	2(1)	3(1)
C(31)	40(2)	28(1)	24(1)	6(1)	-5(1)	-5(1)
C(32)	42(2)	35(2)	19(1)	3(1)	7(1)	-15(1)
C(33)	27(1)	27(1)	24(1)	-2(1)	6(1)	-5(1)
C(34)	28(1)	14(1)	17(1)	0(1)	4(1)	-3(1)
C(35)	27(1)	37(2)	22(1)	2(1)	8(1)	-4(1)
C(36)	40(2)	38(2)	19(1)	-2(1)	2(1)	-9(1)
C(37)	57(2)	23(1)	15(1)	-3(1)	16(1)	-5(1)
C(38)	42(2)	24(1)	31(2)	1(1)	24(1)	3(1)
C(39)	31(1)	17(1)	20(1)	2(1)	9(1)	2(1)
C(40)	21(1)	23(1)	14(1)	0(1)	2(1)	0(1)
C(41)	22(1)	27(1)	19(1)	3(1)	6(1)	-1(1)
C(42)	29(2)	29(1)	27(1)	-2(1)	7(1)	10(1)
C(43)	35(2)	21(1)	37(2)	-4(1)	7(1)	1(1)
C(44)	38(2)	25(1)	50(2)	0(1)	22(2)	-7(1)
C(45)	28(1)	25(1)	35(2)	-6(1)	17(1)	-3(1)
C(46)	16(1)	26(1)	18(1)	8(1)	2(1)	1(1)
C(47)	22(1)	24(1)	18(1)	5(1)	-2(1)	0(1)
C(48)	28(1)	28(1)	25(1)	4(1)	2(1)	-7(1)
C(49)	22(1)	38(2)	30(2)	10(1)	6(1)	-8(1)
C(50)	26(1)	38(2)	24(1)	8(1)	9(1)	5(1)
C(51)	19(1)	27(1)	20(1)	5(1)	4(1)	2(1)
C(52)	25(1)	36(2)	31(2)	-2(1)	9(1)	2(1)
C(53)	27(2)	27(1)	28(1)	-2(1)	3(1)	-5(1)

Table 5.
Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for BP3CoOAr.

	x	y	z	U(eq)
H(2)	10437	7476	1287	28
H(3)	11659	7817	1084	34
H(4)	11663	8556	-111	35
H(5)	10407	8923	-1141	36

H(6)	9185	8582	-933	32
H(7A)	8077	8891	-330	22
H(7B)	8733	9158	562	22
H(8A)	8430	6659	-267	24
H(8B)	8372	7358	-951	24
H(9A)	9165	7821	1759	24
H(9B)	9384	6990	1393	24
H(11)	5777	9092	323	30
H(12)	4900	10188	-210	37
H(13)	5424	11409	-521	41
H(14)	6826	11536	-292	39
H(15)	7700	10443	221	32
H(17)	6908	9040	2126	31
H(18)	7420	9456	3552	38
H(19)	8810	9776	4158	36
H(20)	9679	9657	3353	36
H(21)	9151	9260	1910	31
H(23)	5974	6801	-2406	31
H(24)	5562	5592	-3148	35
H(25)	6068	4357	-2510	32
H(26)	7015	4339	-1129	33
H(27)	7436	5544	-380	31
H(29)	5821	8373	-1061	30
H(30)	5265	9375	-2084	39
H(31)	5851	9637	-3142	41
H(32)	6970	8896	-3195	40
H(33)	7542	7889	-2177	32
H(35)	9452	7044	3122	35
H(36)	9587	7246	4560	41
H(37)	8420	7399	4965	37
H(38)	7120	7313	3931	35
H(39)	6987	7113	2483	27
H(41)	9108	5796	882	28
H(42)	9160	4388	754	34
H(43)	8347	3556	1273	39
H(44)	7473	4130	1931	43
H(45)	7370	5527	2017	33
H(48)	4454	5445	778	35
H(49)	3858	5970	1740	37
H(50)	4292	7205	2393	35
H(52A)	5359	8685	1791	46
H(52B)	5985	8214	2587	46
H(52C)	5074	8410	2581	46
H(53A)	5459	6385	-331	43
H(53B)	5418	5493	37	43
H(53C)	6209	6051	457	43